```
=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sam sss
MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE

=> s l1
MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE

=> file casreact
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 2.30       2.51

FILE 'CASREACT' ENTERED AT 18:40:21 ON 03 AUG 2008
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FILE CONTENT:1840 - 3 Aug 2008 VOL 149 ISS 6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 15.3 million reactions     *
*                                                           *
*************************************************************

In addition to reactions indexed by CAS, CASREACT contains reactions
derived from the following: ZIC/VINITI database (1974-1999) provided
by InfoChem; INPI data prior to 1986; Biotransformations database
compiled under the direction of Professor Dr. Klaus Kieslich; organic
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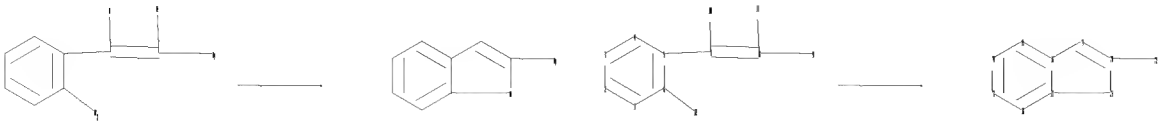
This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Documents and Settings\EBernhardt\My
Documents\Stnexp\Queries\10557537-II.str
```



chain nodes :
7 8 9 10 11 12 22
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18 19 20 21
chain bonds :
5-7 6-12 7-8 7-10 8-9 8-11 20-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 16-19 17-18
17-21 19-20 20-21
exact/norm bonds :
8-9 16-19 17-21 19-20 20-21 20-22
exact bonds :
5-7 6-12 7-8 7-10 8-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom
Generic attributes :
9:
Saturation : Unsaturated
22:
Saturation : Unsaturated

fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1

L2 STRUCTURE UPLOADED

=> s l2
SAMPLE SEARCH INITIATED 18:40:57 FILE 'CASREACT'
SCREENING COMPLETE - 493 REACTIONS TO VERIFY FROM 56 DOCUMENTS

100.0% DONE 493 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 8529 TO 11191
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2 (0 REACTIONS)

=> s l2 sss full
FULL SEARCH INITIATED 18:41:06 FILE 'CASREACT'
SCREENING COMPLETE - 13464 REACTIONS TO VERIFY FROM 1374 DOCUMENTS

100.0% DONE 13464 VERIFIED 88 HIT RXNS 18 DOCS
SEARCH TIME: 00.00.05

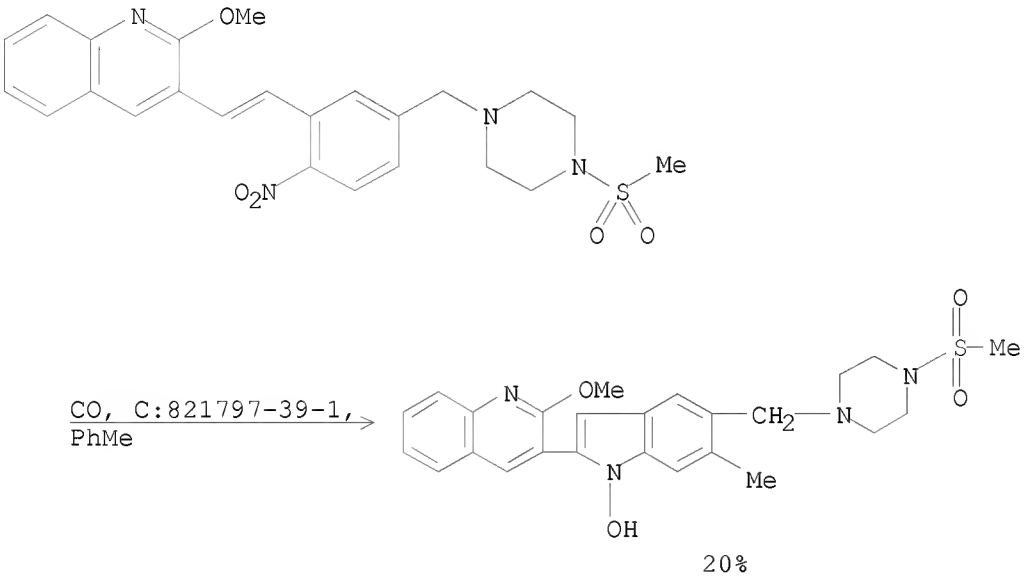
L4 18 SEA SSS FUL L2 (88 REACTIONS)

=> d scan 1-18
'1-18' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Substituted indoles and a process for their preparation via Pd/diamine-catalyzed reductive cyclization of ortho-nitrostyrenes under CO pressure

RX(5) OF 30



20%

NOTE: Endeavor reactor was used

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels

IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,

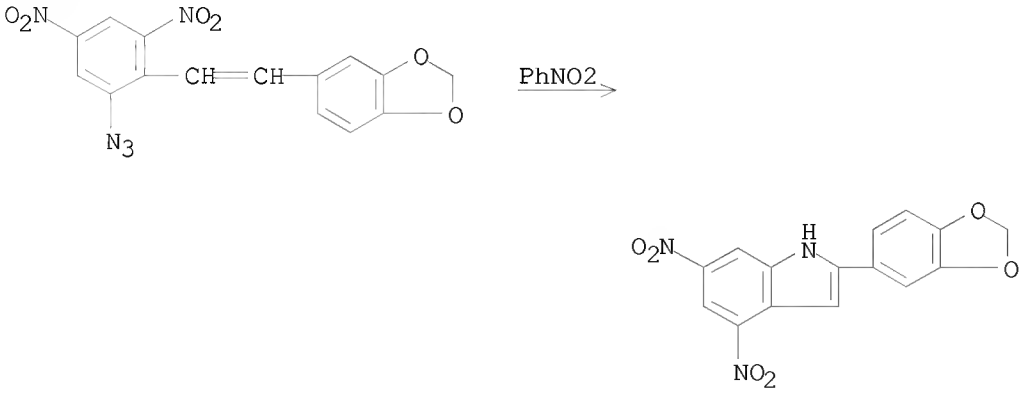
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):17

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2-aryl- and 2-hetaryl-4,6-dinitroindoles from 2,4,6-trinitrotoluene

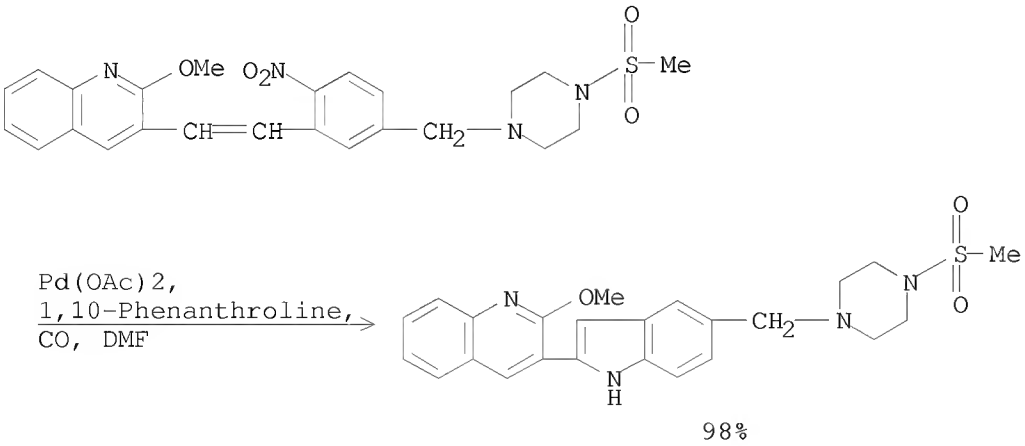
RX(22) OF 57



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI A highly active catalyst for the reductive cyclization of ortho-nitrostyrenes under mild conditions

RX(1) OF 47

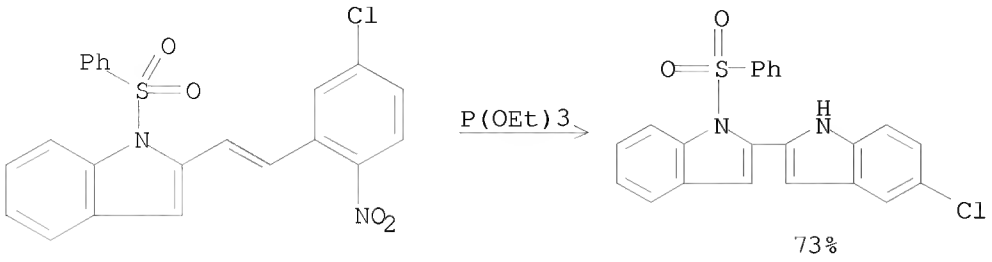


NOTE: optimization study, green chem. - waste reduction

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Effective Strategy for the Preparation of Indolocarbazole Aglycons and Glycosides: Total Synthesis of Tjipanazoles B, D, E, and I

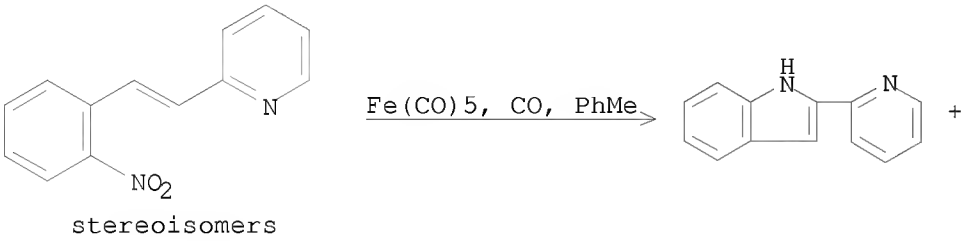
RX(3) OF 71



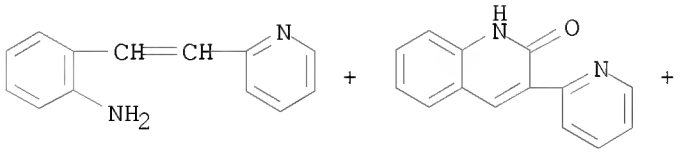
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Deoxygenation reactions of ortho-nitrostyrenes with carbon monoxide catalyzed by metal carbonyls: a new route to indoles

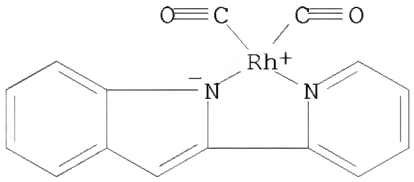
RX(8) OF 12



stereoisomers



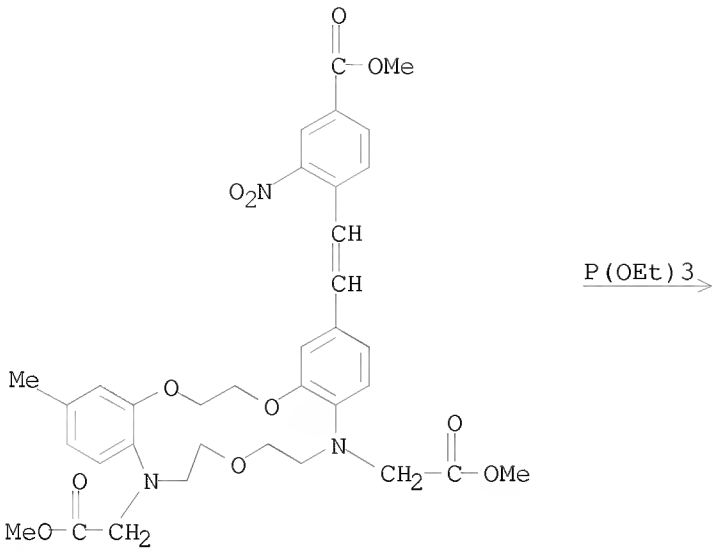
RX(8) OF 12



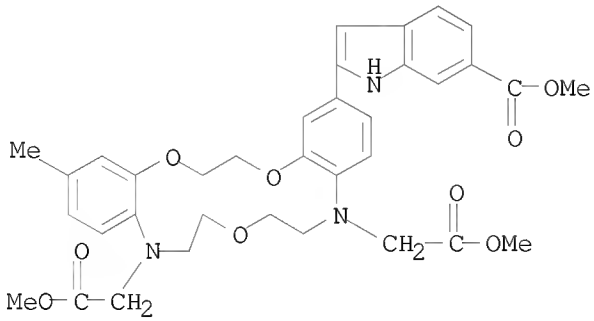
L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Preparation of crown ether derivatives as metal chelating agents

RX(26) OF 555



RX(26) OF 555

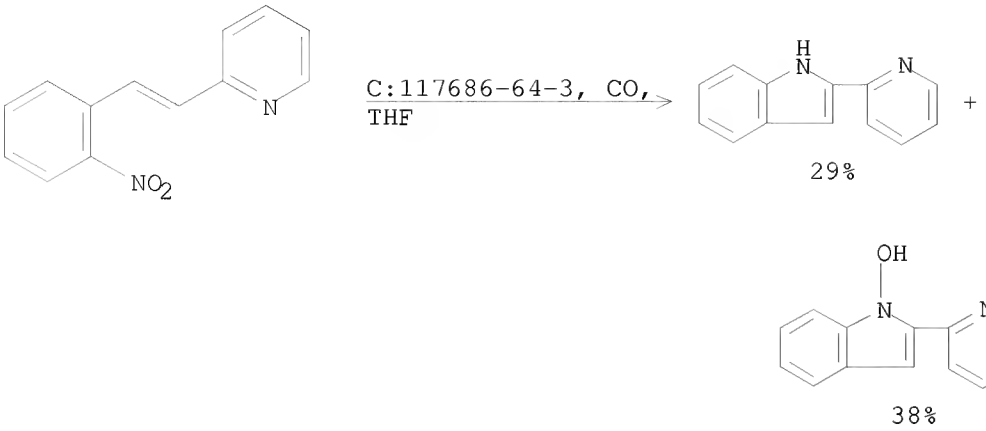


80%

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI The unprecedented detection of the intermediate formation of N-hydroxy derivatives during the carbonylation of 2'-nitrochalcones and 2-nitrostyrenes catalyzed by palladium

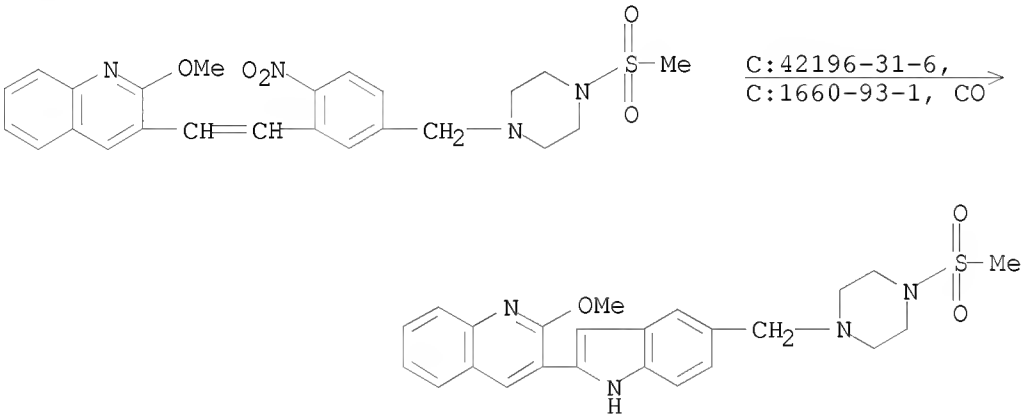
RX(4) OF 5



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Applying statistical design of experiments and automation to the rapid optimization of metal-catalyzed processes in process development

RX(2) OF 2

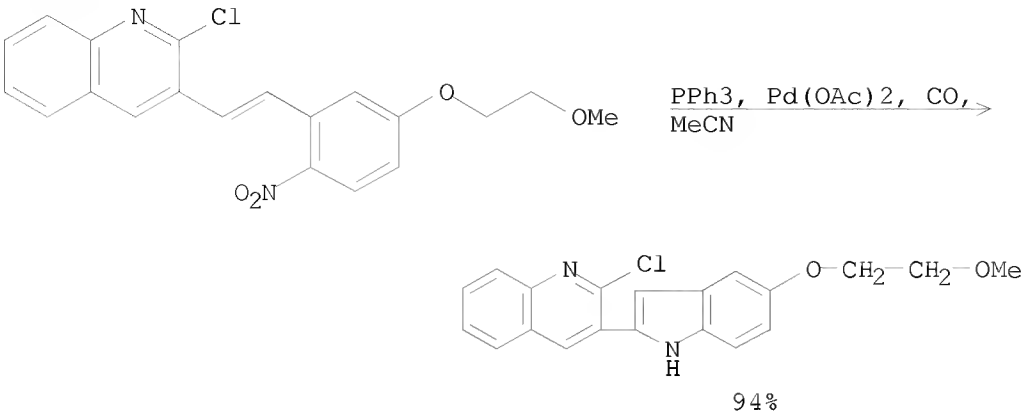


NOTE: optimization study, optimized on catalyst loading, optimized on pressure, optimized on temperature

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Rapid and Efficient Synthesis of 1H-Indol-2-yl-1H-quinolin-2-ones

RX(4) OF 63

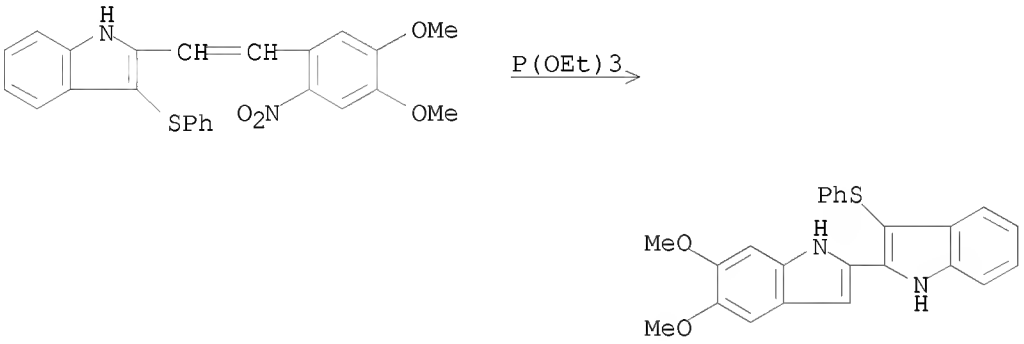


NOTE: alternative prepn. shown

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2,2'-biindolyls; potential intermediates for indolocarbazole alkaloids

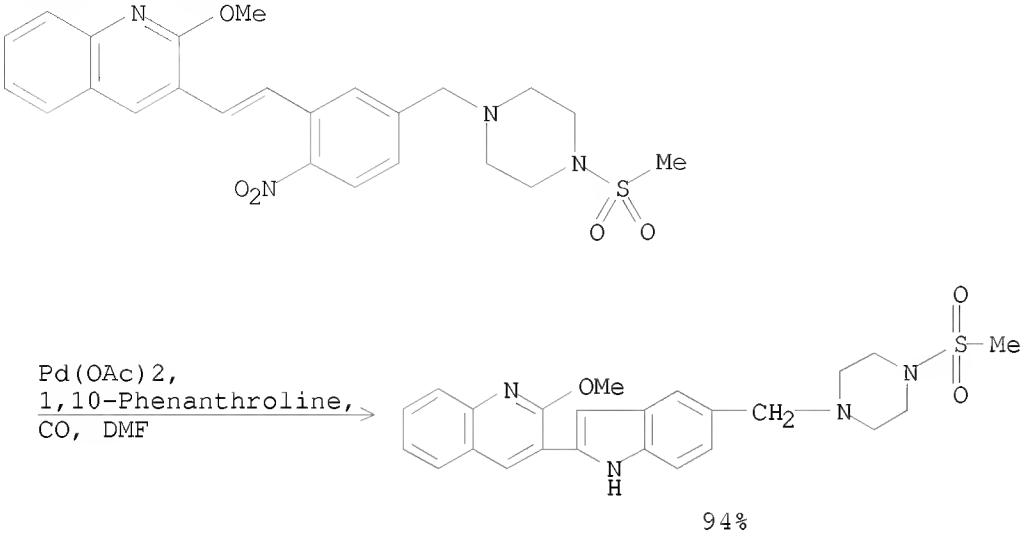
RX(2) OF 6



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 5-Substituted-1H-indol-2-yl-1H-quinolin-2-ones: A Novel Class of KDR Kinase Inhibitors

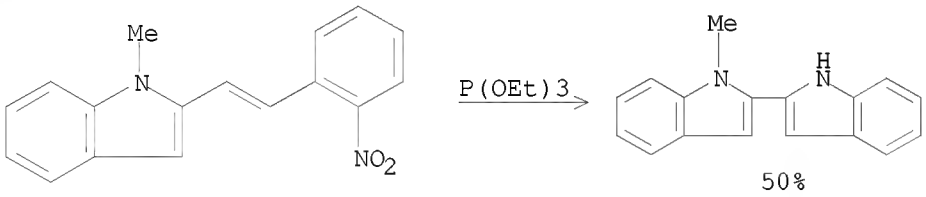
RX(36) OF 350



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Benzannulation reactions of Fischer carbene complexes for the synthesis of indolocarbazoles

RX(10) OF 177

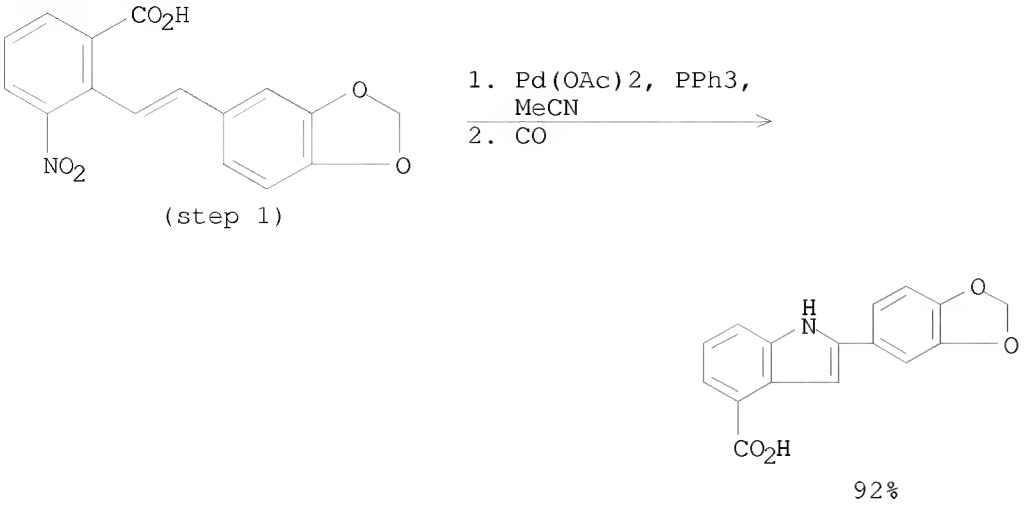


NOTE: thermal, alternative prepns. gave similar yields

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Preparation of 2-arylindole-4-carboxylic amide derivatives

RX(15) OF 47



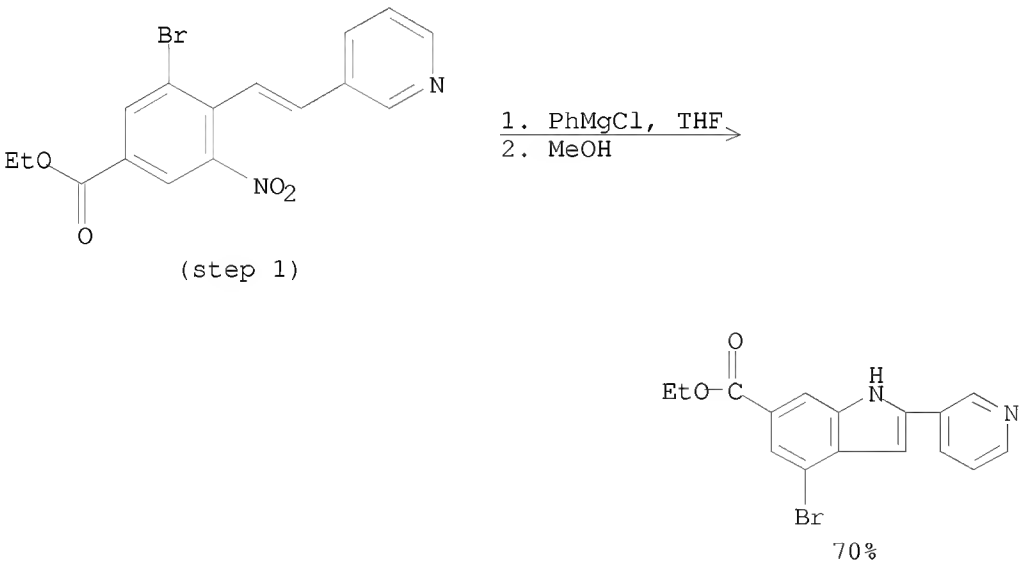
(step 1)

92%

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Mild synthesis of polyfunctional benzimidazoles and indoles by the reduction of functionalized nitroarenes with phenylmagnesium chloride

RX(37) OF 85



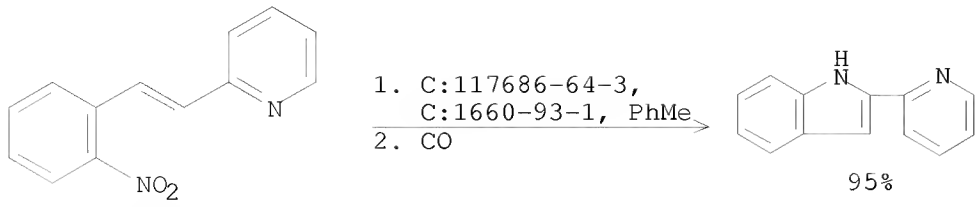
(step 1)

70%

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of 2-heteroaryl-substituted indoles via palladium-catalyzed reductive N-heterocyclization

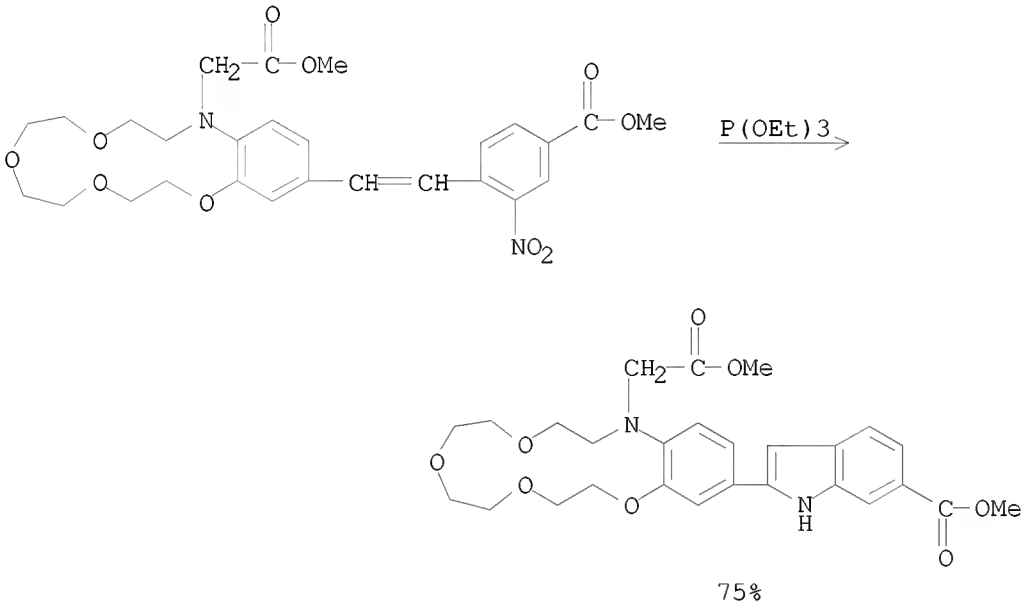
RX(1) OF 9



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Fluorescent metal ion indicators based on benzoannelated crown systems: a green fluorescent indicator for intracellular sodium ions

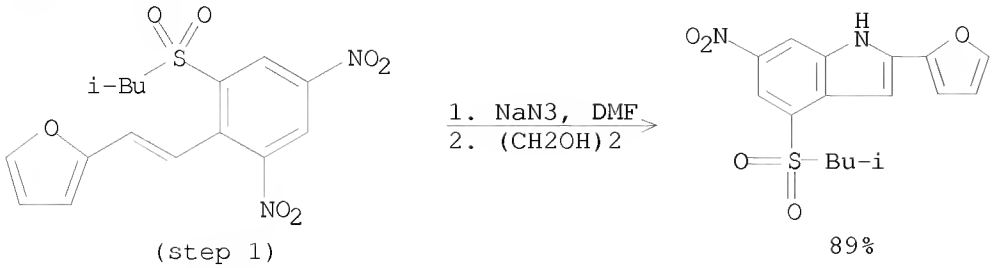
RX(28) OF 161



L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Interaction of 2,4,6-trinitrotoluene and its analogs with aldehydes. Synthesis of benzo-annelated heterocycles from the products of condensation

RX(11) OF 29



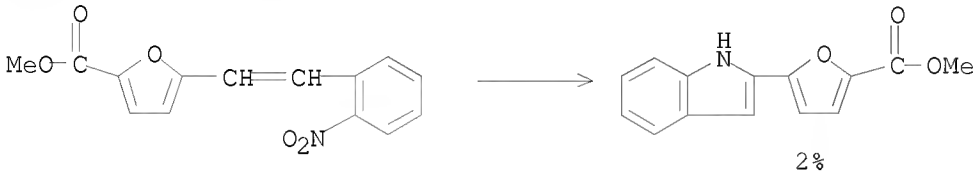
(step 1) 89%

NOTE: regioselective, thermal, stereoselective

L4 18 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Intramolecular ring formation of phenyl azide and furan moieties

RX(69) OF 98 - 3 STEPS



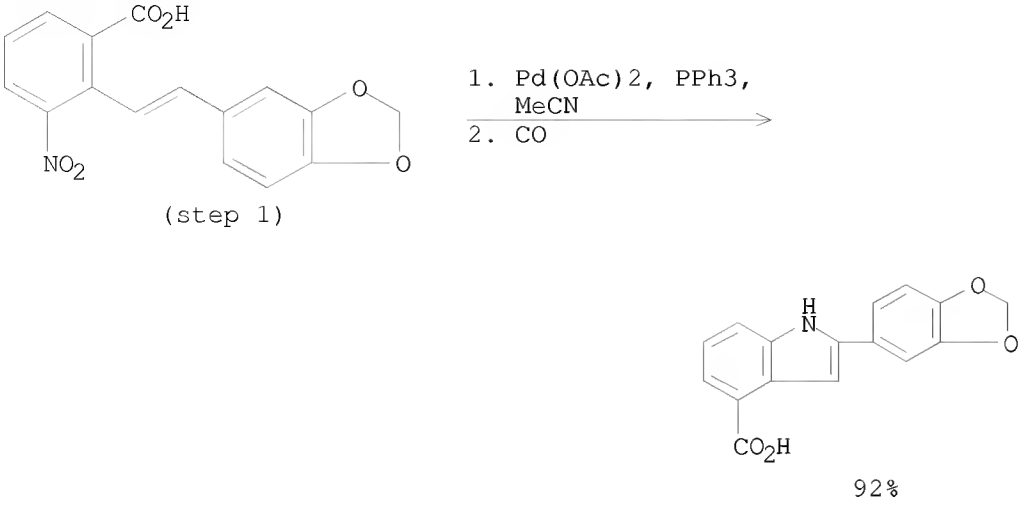
2%

ALL ANSWERS HAVE BEEN SCANNED

=> d crd

L4 ANSWER 1 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(15) OF 47

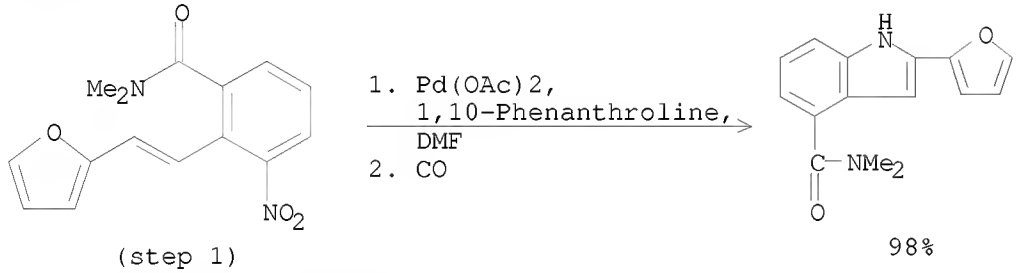


(step 1)

92%

CON: STAGE(1) room temperature -> 70 deg C
STAGE(2) 16 hours, 70 deg C, 60 psi

RX(23) OF 47

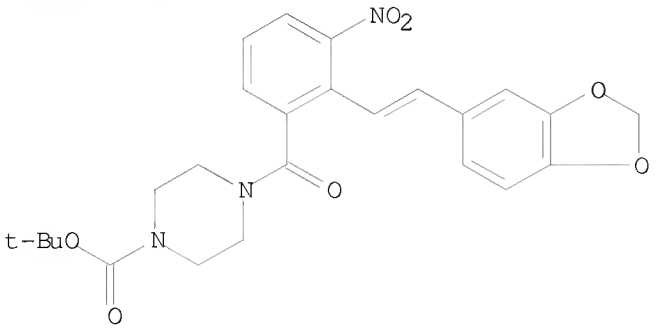


(step 1)

98%

CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

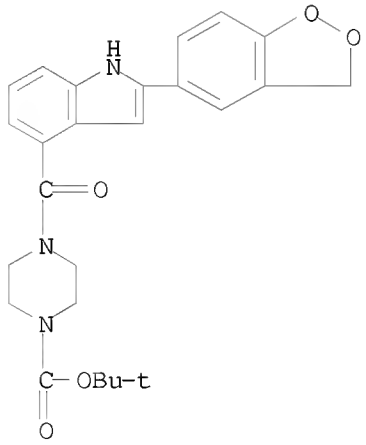
RX(25) OF 47



(step 1)

1. Pd(OAc)2, 1,10-Phenanthroline, DMF
2. CO

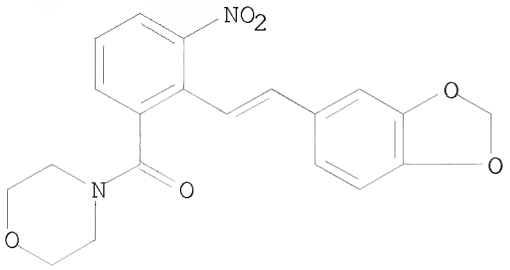
RX(25) OF 47



99%

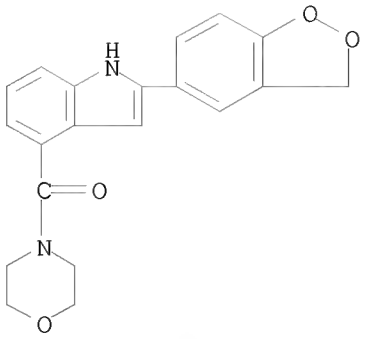
CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(27) OF 47



(step 1)

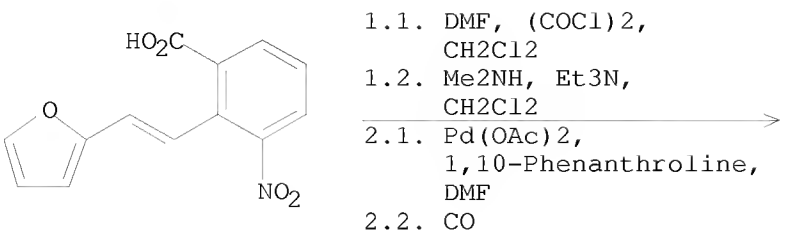
1. Pd(OAc)2, 1,10-Phenanthroline, DMF
2. CO



98%

CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

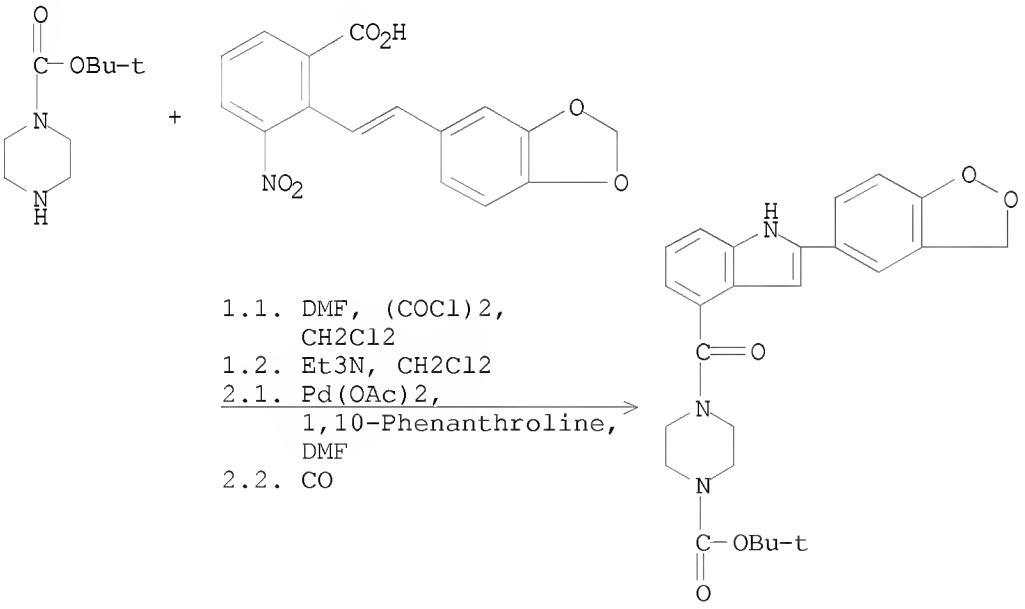
RX(37) OF 47 - 2 STEPS



98%

CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

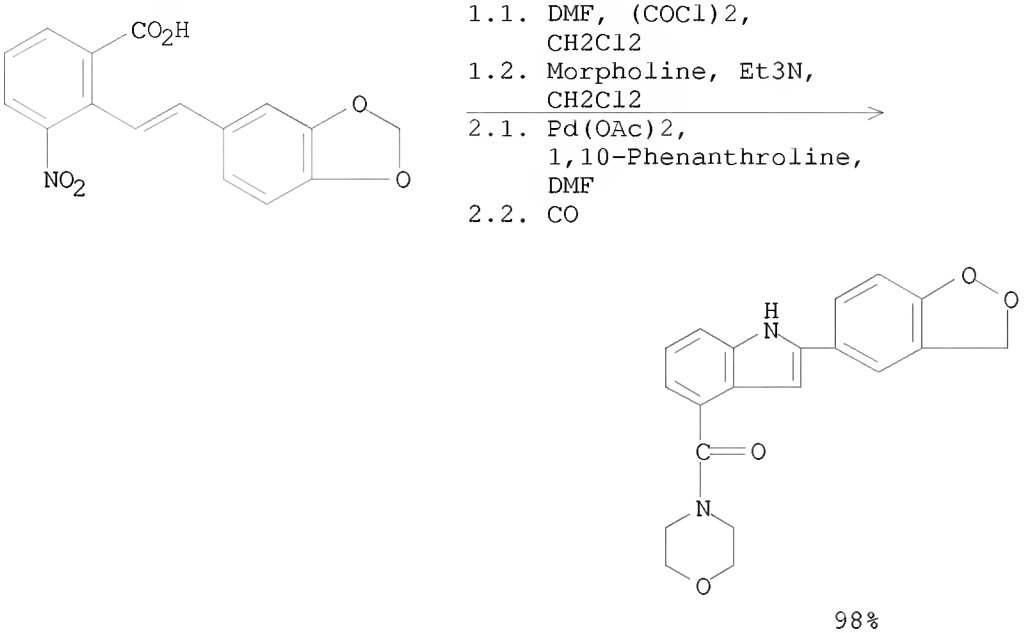
RX(39) OF 47 - 2 STEPS



99%

CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(41) OF 47 - 2 STEPS



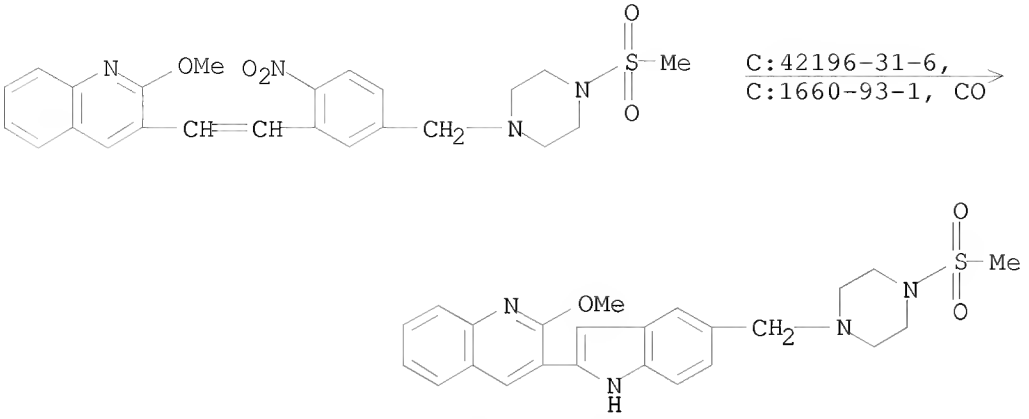
98%

CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

=> d crd 2-18

L4 ANSWER 2 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

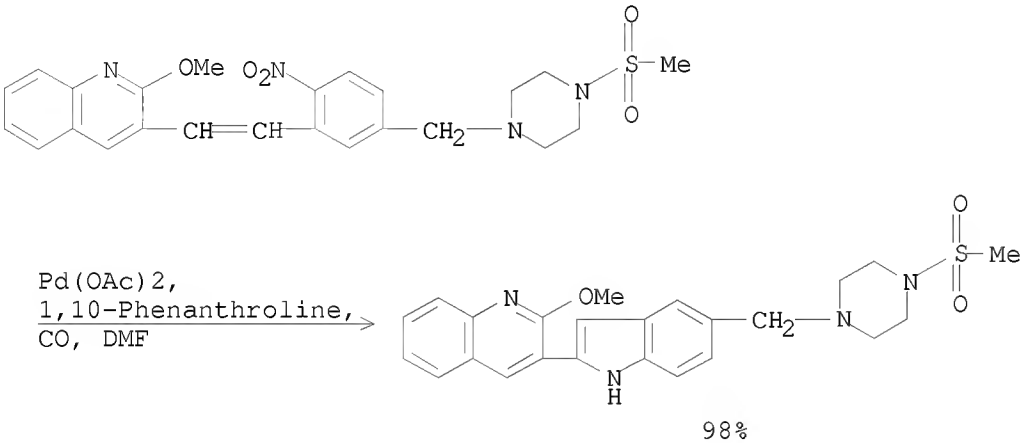
RX(2) OF 2



NOTE: optimization study, optimized on catalyst loading, optimized on pressure, optimized on temperature
CON: 70 - 80 deg C, 15 psi

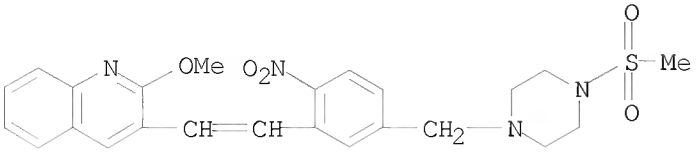
L4 ANSWER 3 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

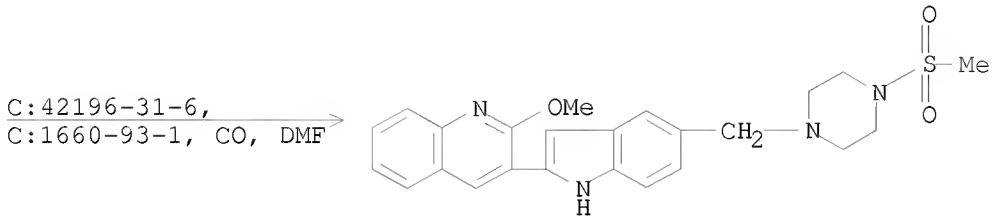
RX(1) OF 47



NOTE: optimization study, green chem. - waste reduction
CON: 70 deg C, 15 psi

RX(2) OF 47

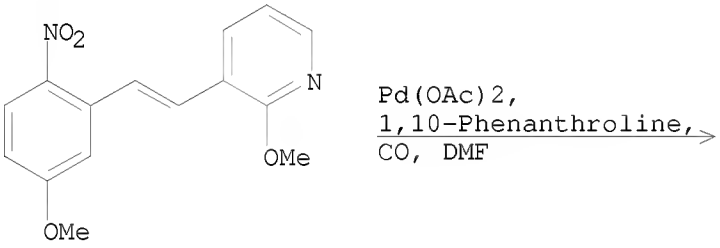


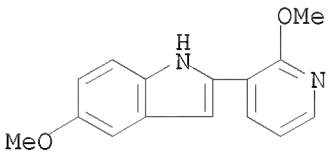


100%

NOTE: optimization study, green chem. - waste reduction
CON: 70 deg C, 15 psi

RX(23) OF 47

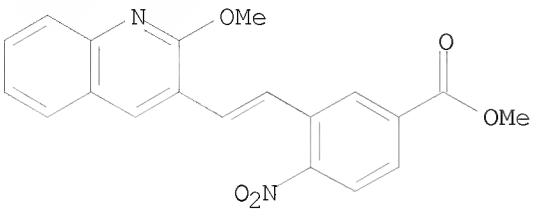




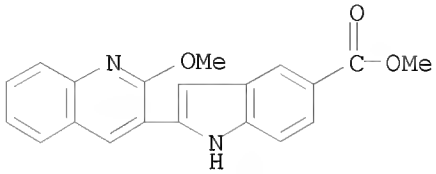
72%

NOTE: green chem. - waste reduction
CON: 16 hours, 70 deg C, 30 psi

RX(24) OF 47



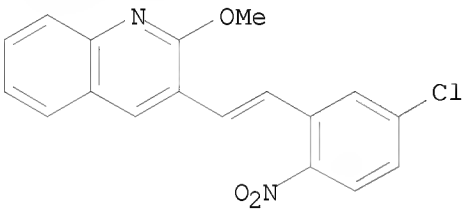
C:42196-31-6,
C:1660-93-1, CO, DMF



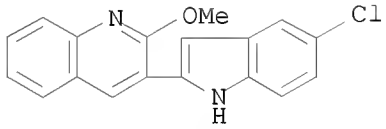
78%

NOTE: green chem. - waste reduction
CON: 16 hours, 80 deg C, 15 psi

RX(25) OF 47



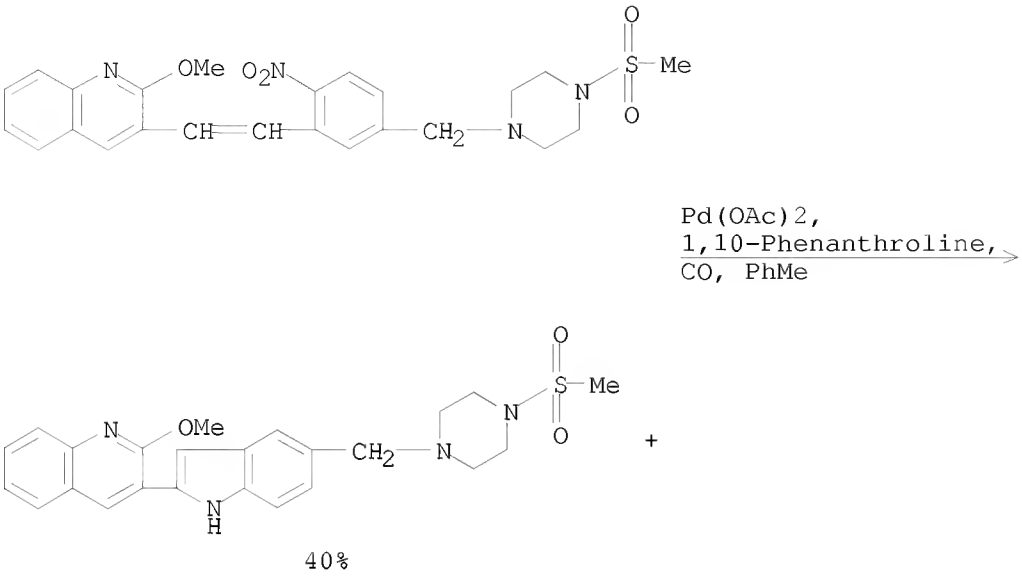
Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF



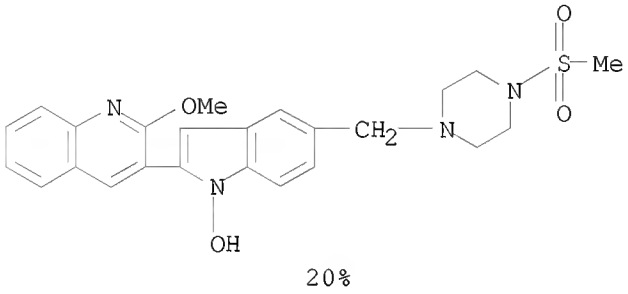
91%

NOTE: green chem. - waste reduction
CON: 16 hours, 80 deg C, 15 psi

RX(28) OF 47



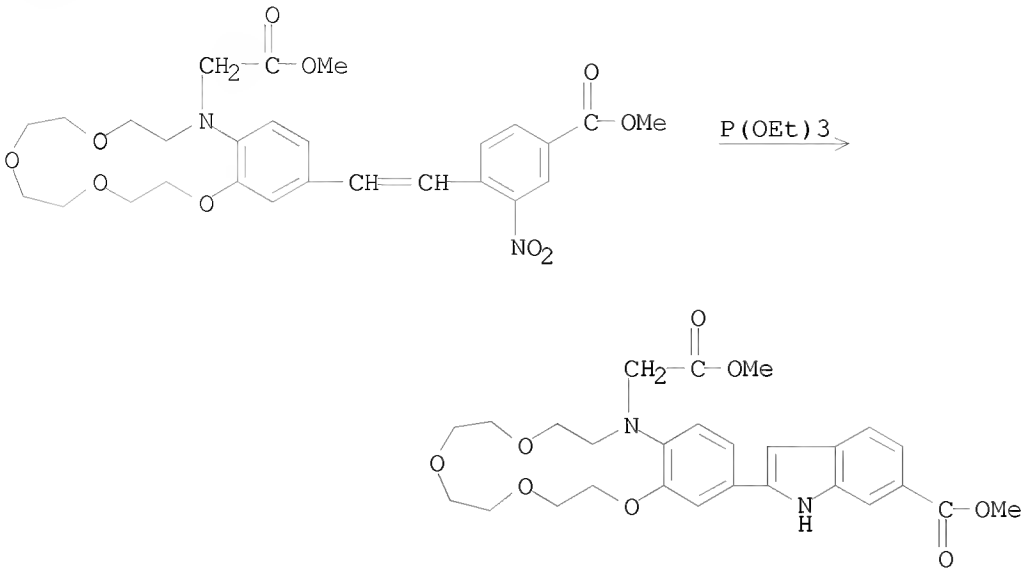
RX(28) OF 47



CON: 70 deg C, 15 psi

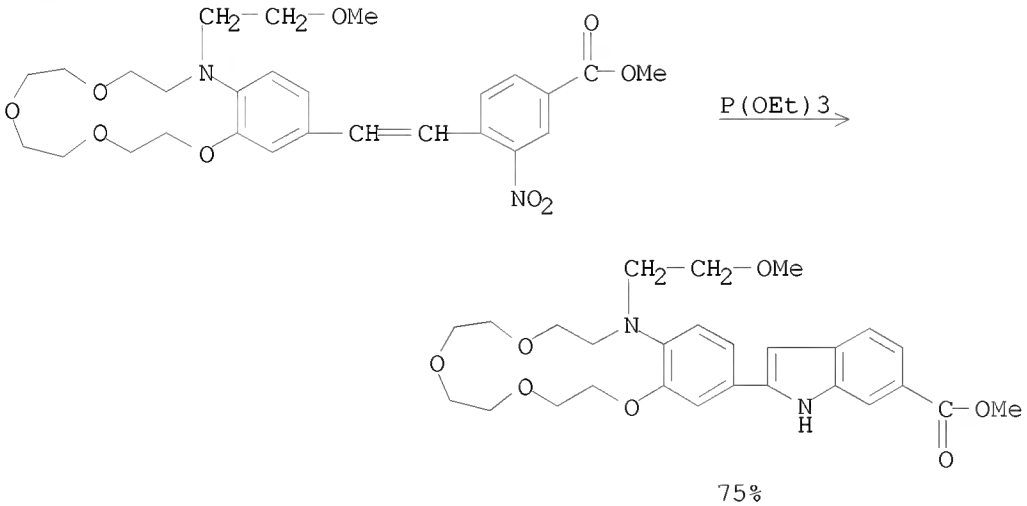
L4 ANSWER 4 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(28) OF 161



75%

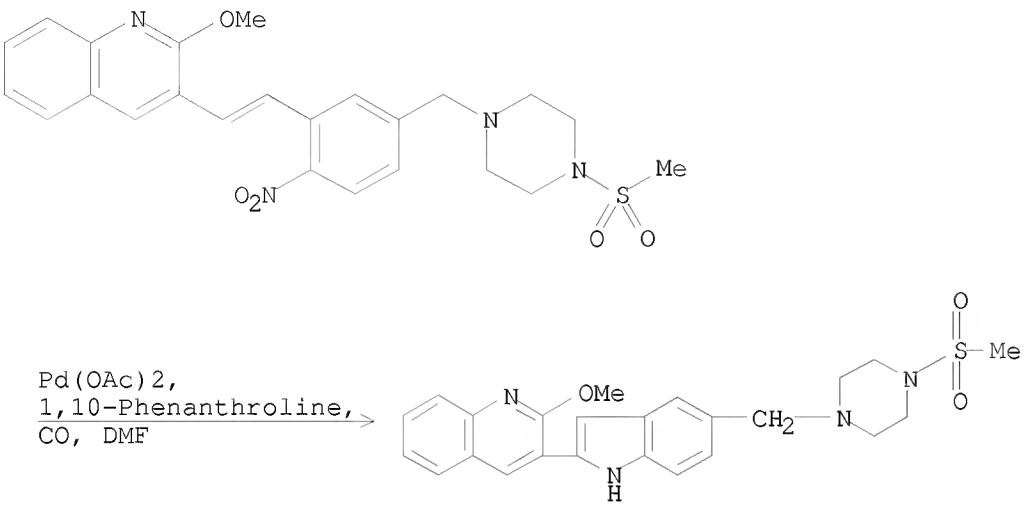
RX(29) OF 161



75%

L4 ANSWER 5 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

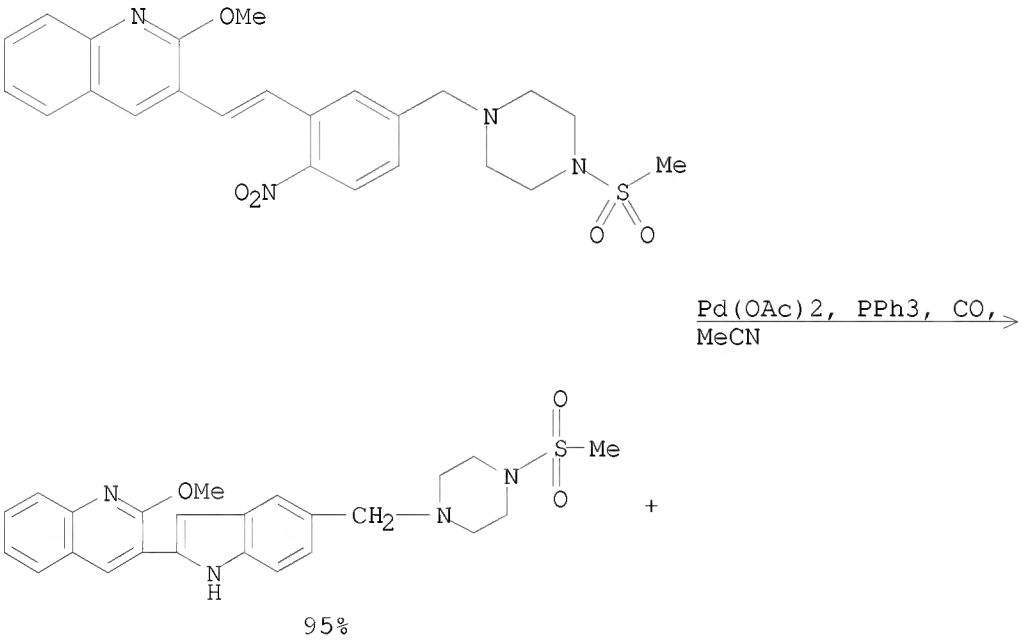
RX(36) OF 350



94%

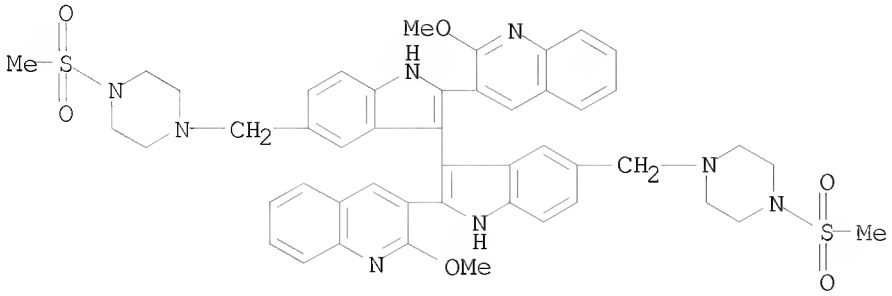
CON: 14 hours, 70 deg C, 15 psi

RX(37) OF 350



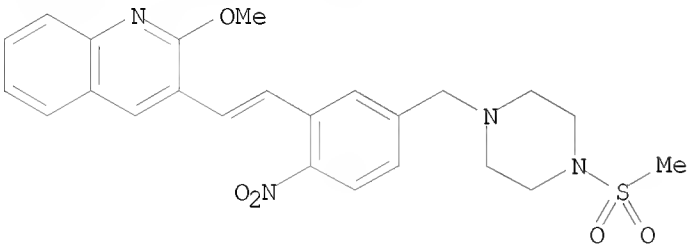
95%

RX(37) OF 350



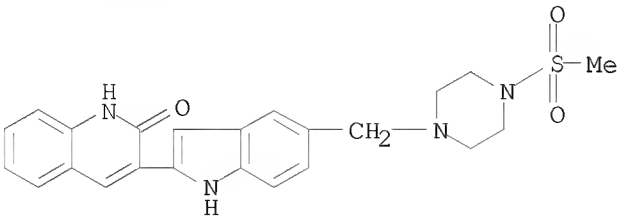
CON: 15 hours, 70 deg C, 60 atm

RX(59) OF 350 - 2 STEPS



1. Pd(OAc)2,
   1,10-Phenanthroline,
   CO, DMF
2. HCl, Water, DMF

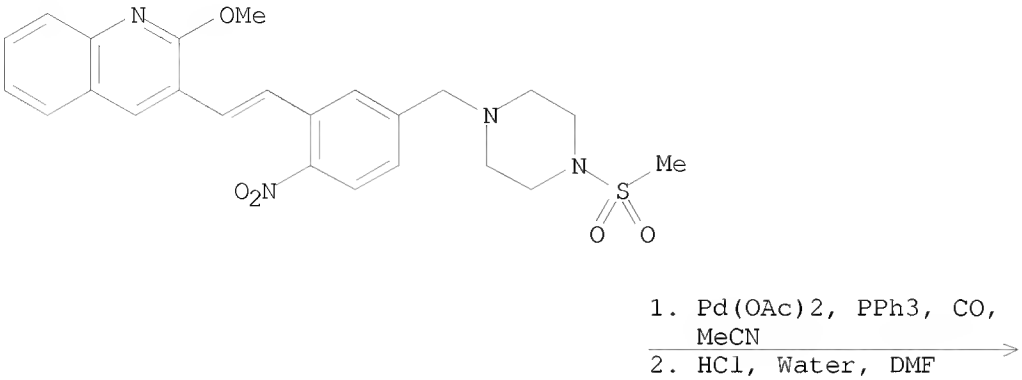
RX(59) OF 350 - 2 STEPS



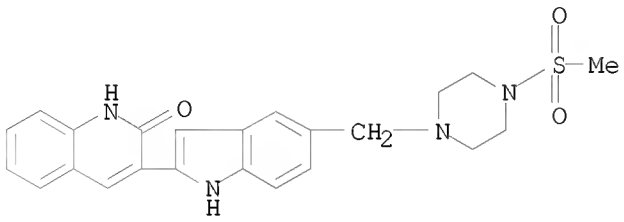
HCl
100%

CON: STEP(1) 14 hours, 70 deg C, 15 psi

RX(60) OF 350 - 2 STEPS



RX(60) OF 350 - 2 STEPS

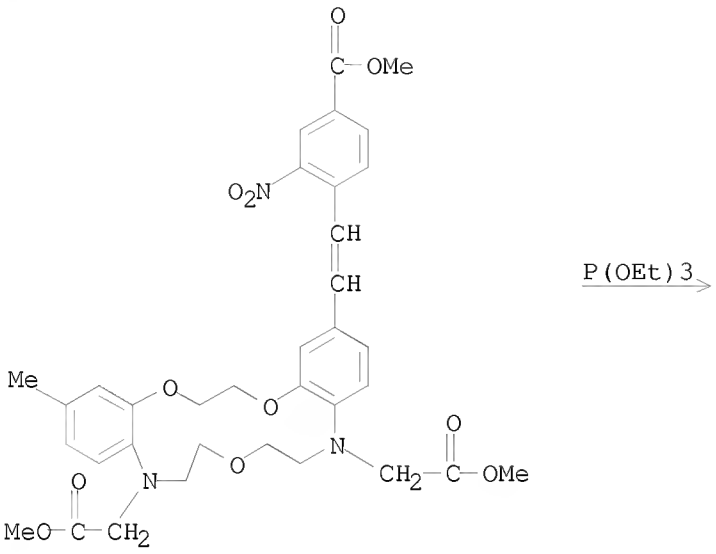


HCl
100%

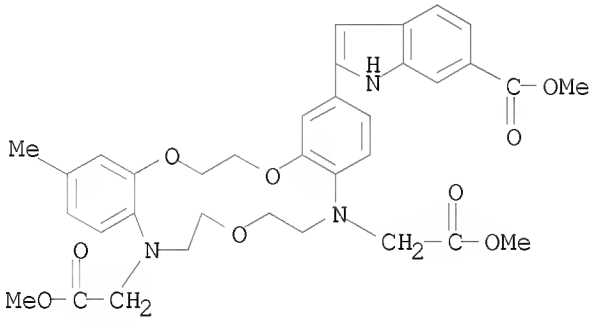
CON: STEP(1) 15 hours, 70 deg C, 60 atm

L4 ANSWER 6 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(26) OF 555



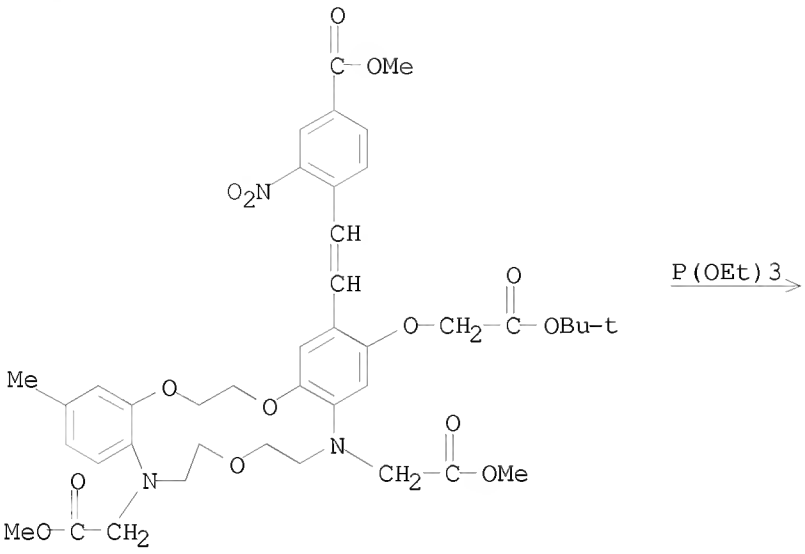
RX(26) OF 555



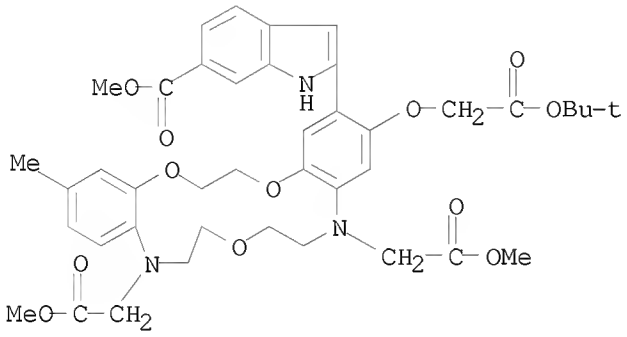
80%

CON: 6 hours, 120 deg C

RX(48) OF 555



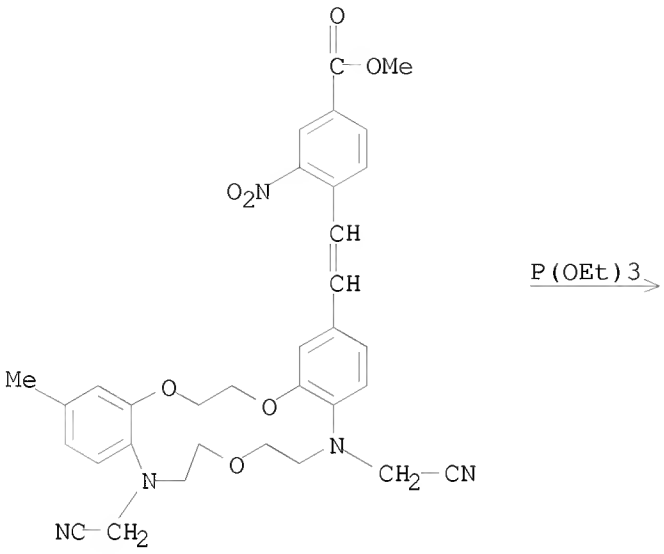
RX(48) OF 555



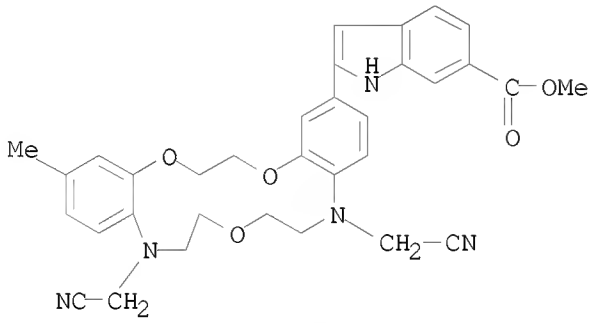
34%

CON: 7 hours, 130 deg C

RX(54) OF 555



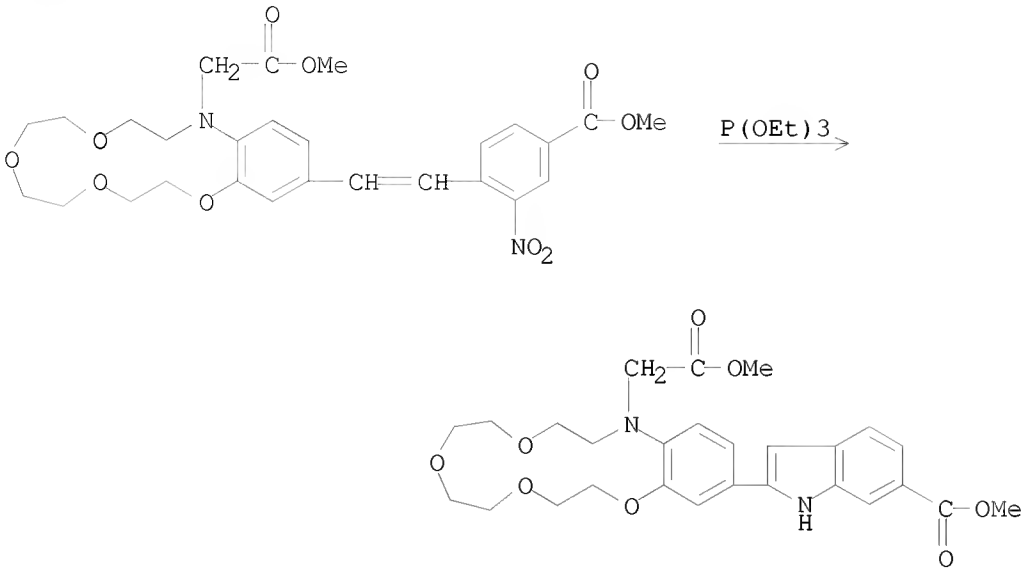
RX(54) OF 555



16%

CON: 16 hours, 120 deg C

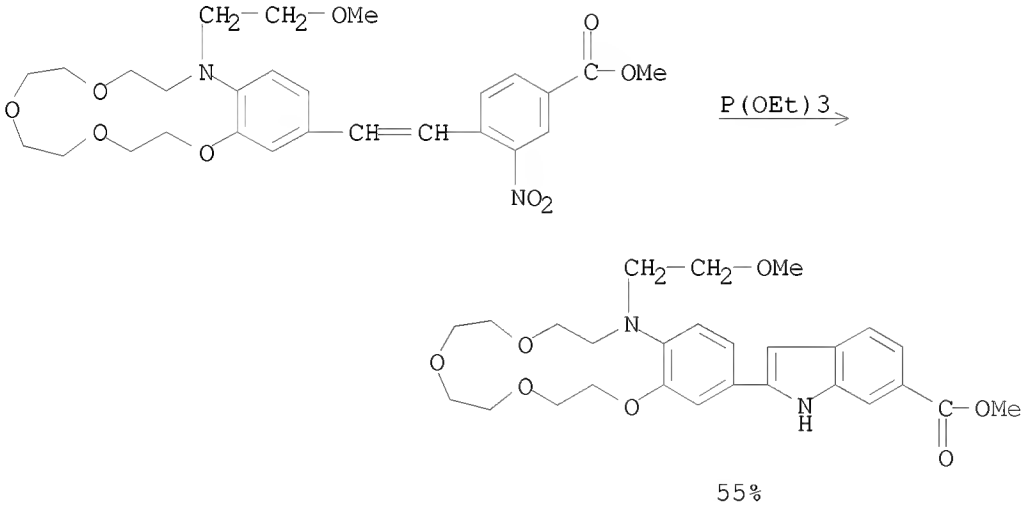
RX(67) OF 555



34%

CON: 4 hours, 125 deg C

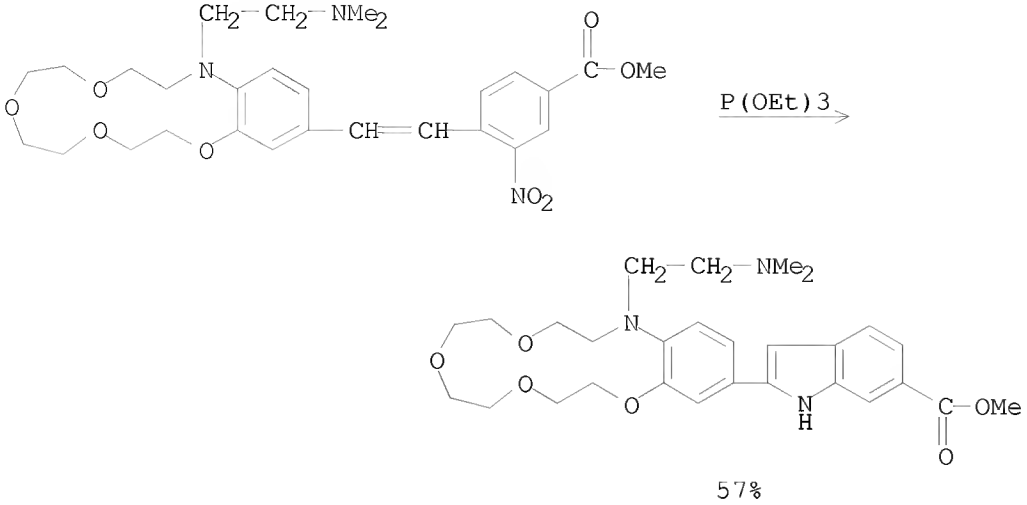
RX(91) OF 555



55%

CON: 4 hours, 125 deg C

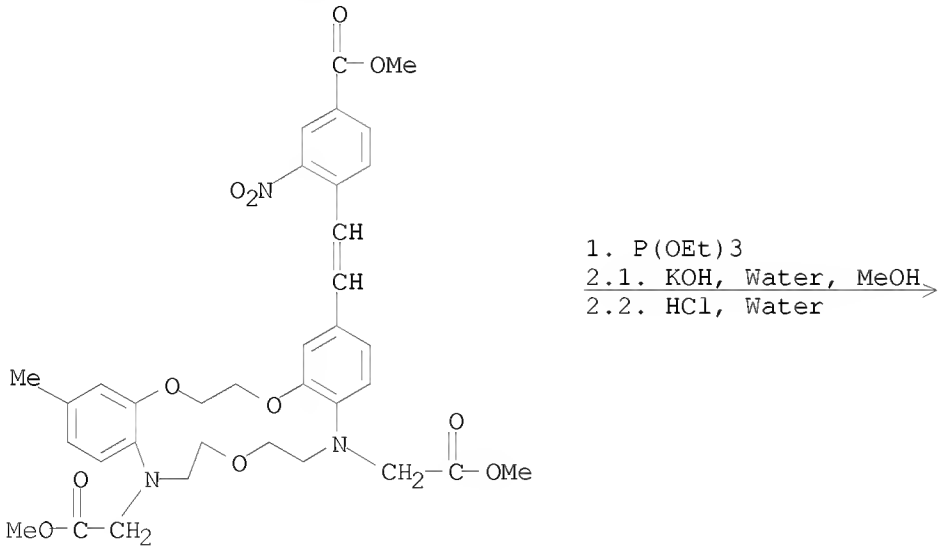
RX(97) OF 555



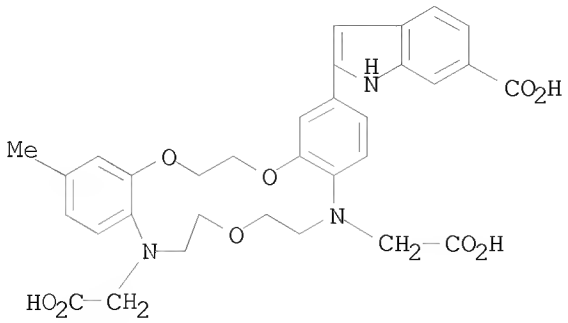
57%

CON: 14 hours, 125 deg C

RX(132) OF 555 - 2 STEPS



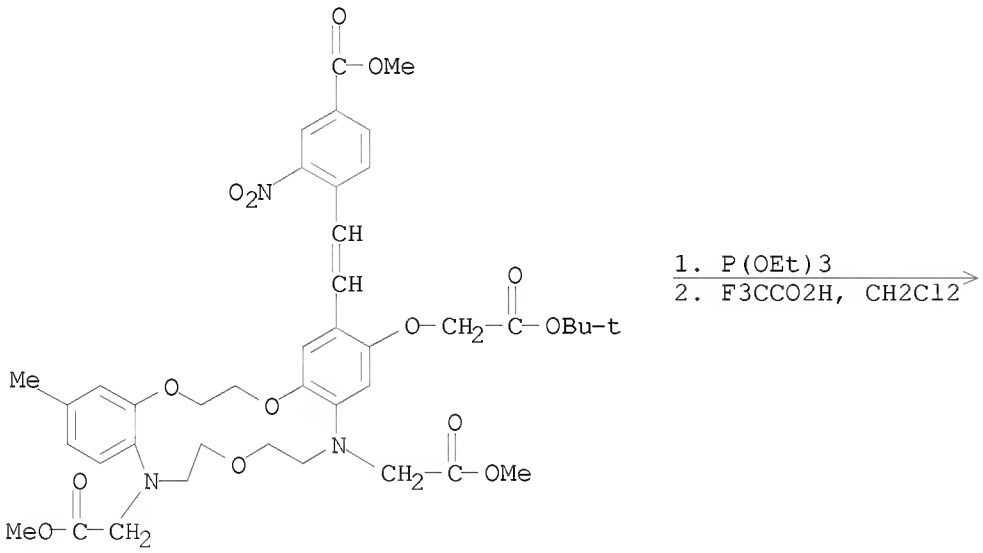
RX(132) OF 555 - 2 STEPS



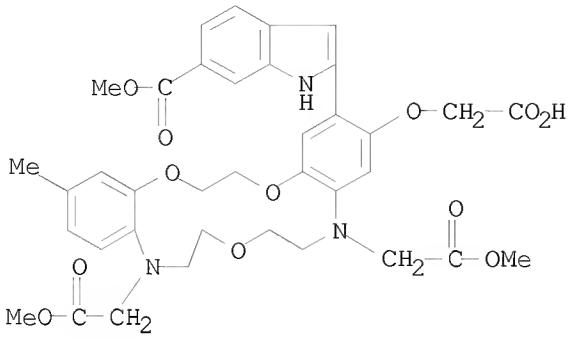
57%

NOTE: 2) incremental addition of reagent in stage 1
CON: STEP(1) 6 hours, 120 deg C
STEP(2.1) 22 hours, room temperature
STEP(2.2) room temperature, pH 3

RX(151) OF 555 - 2 STEPS



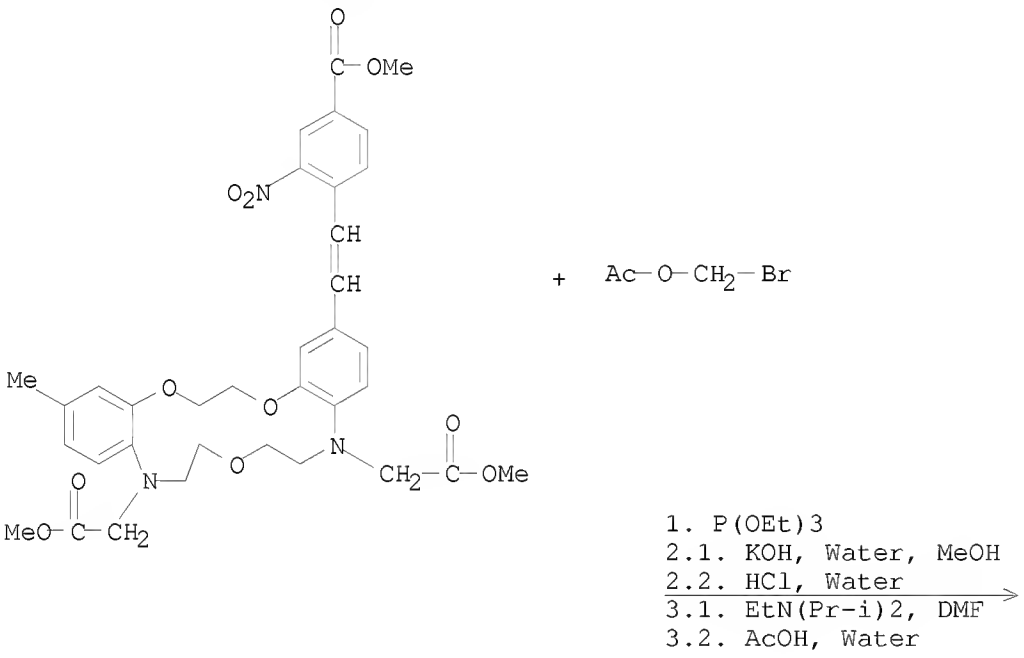
RX(151) OF 555 - 2 STEPS



57%

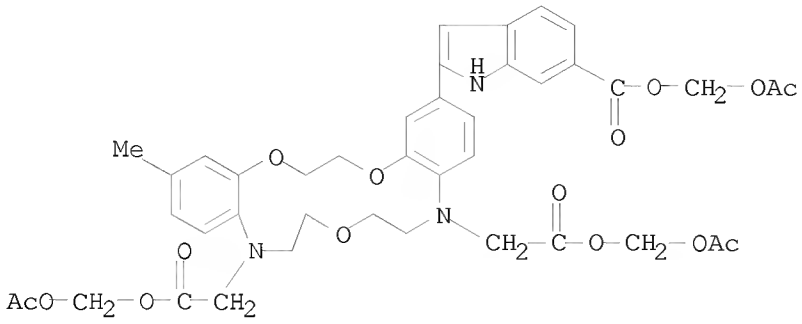
CON: STEP(1) 7 hours, 130 deg C
STEP(2) 3 hours, room temperature

RX(270) OF 555 - 3 STEPS



1. P(OEt)3
2.1. KOH, Water, MeOH
2.2. HCl, Water
3.1. EtN(Pr-i)2, DMF
3.2. AcOH, Water

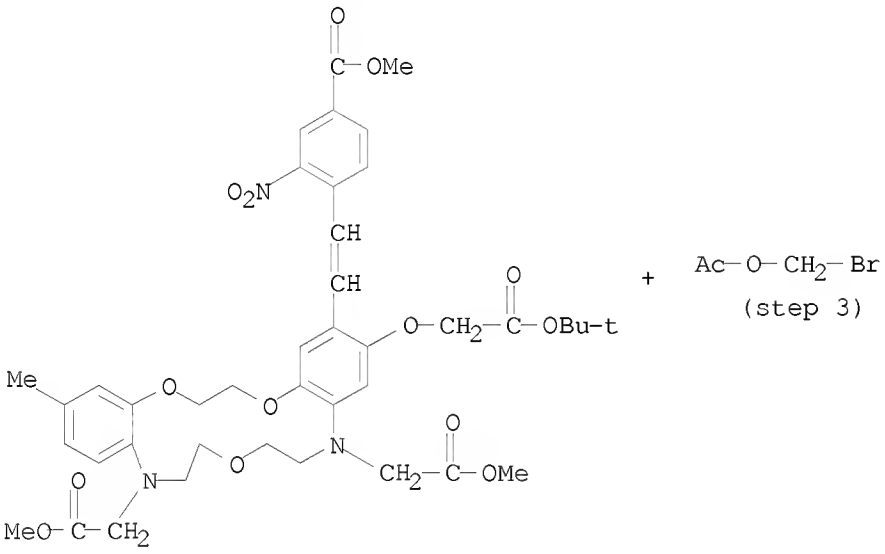
RX(270) OF 555 - 3 STEPS



3%

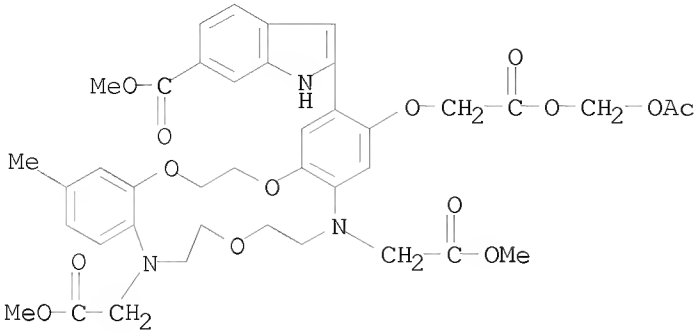
NOTE: 2) incremental addition of reagent in stage 1
CON: STEP(1) 6 hours, 120 deg C
STEP(2.1) 22 hours, room temperature
STEP(2.2) room temperature, pH 3
STEP(3.1) 16 hours, room temperature
STEP(3.2) room temperature

RX(300) OF 555 - 3 STEPS



1. P(OEt)3
2. F3CCO2H, CH2Cl2
3. EtN(Pr-i)2, DMF

RX(300) OF 555 - 3 STEPS

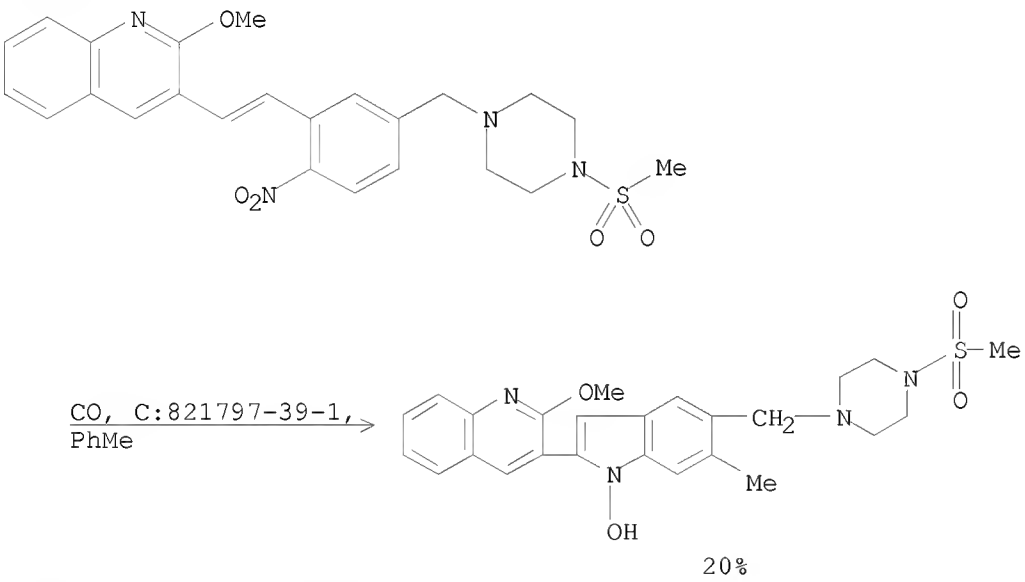


67%

CON: STEP(1) 7 hours, 130 deg C
STEP(2) 3 hours, room temperature
STEP(3) 16 hours, room temperature

L4 ANSWER 7 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

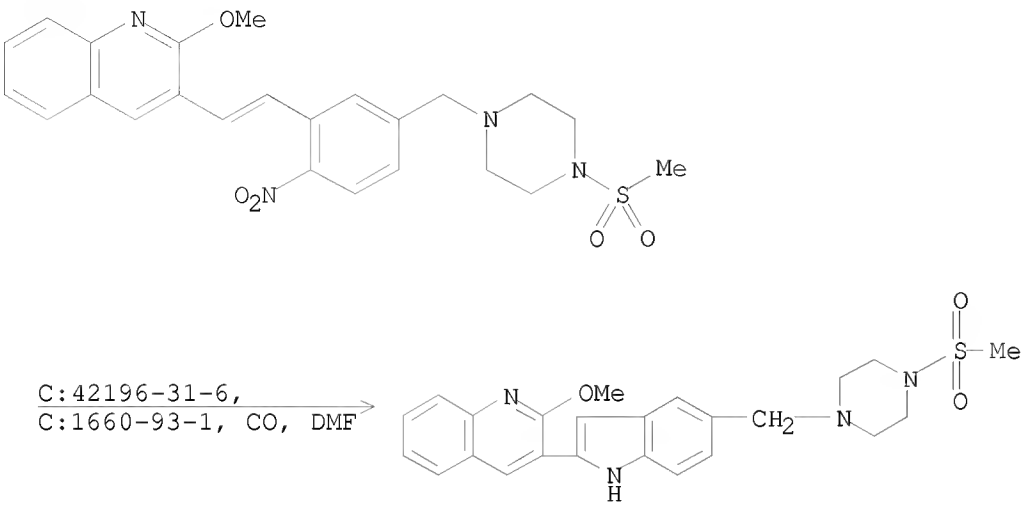
RX(5) OF 30



20%

NOTE: Endeavor reactor was used
CON: STAGE(1) room temperature, 15 psi; 16 hours, 70 deg C

RX(6) OF 30

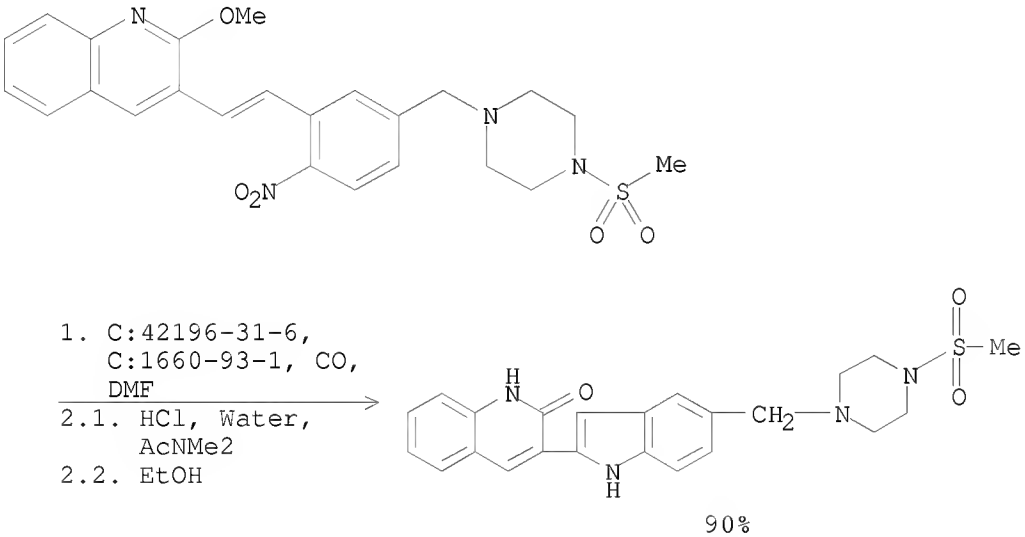


C:42196-31-6,
C:1660-93-1, CO, DMF

83%

CON: STAGE(1) room temperature, 15 psi; 14 hours, 70 deg C

RX(13) OF 30 - 2 STEPS



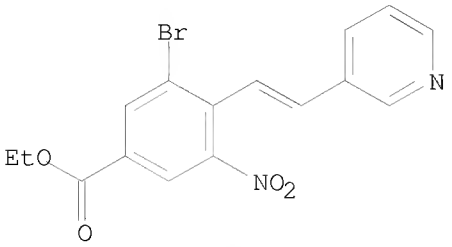
1. C:42196-31-6,
   C:1660-93-1, CO,
   DMF
2.1. HCl, Water,
   AcNMe2
2.2. EtOH

90%

CON: STEP(1.1) room temperature, 15 psi; 14 hours, 70 deg C
STEP(2.1) 2 hours; 60 deg C

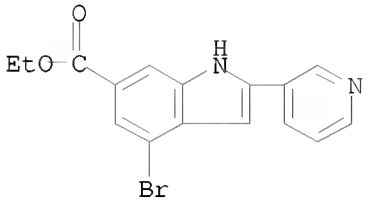
L4 ANSWER 8 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(37) OF 85



1. PhMgCl, THF
2. MeOH

(step 1)

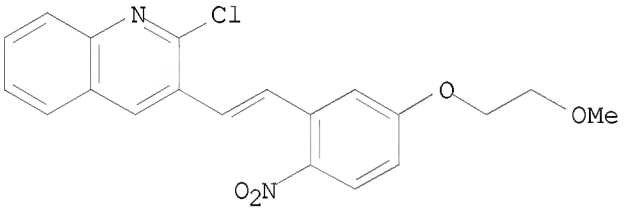


70%

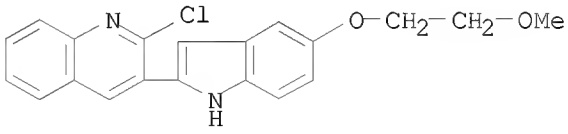
CON: 30 minutes, -40 deg C

L4 ANSWER 9 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 63



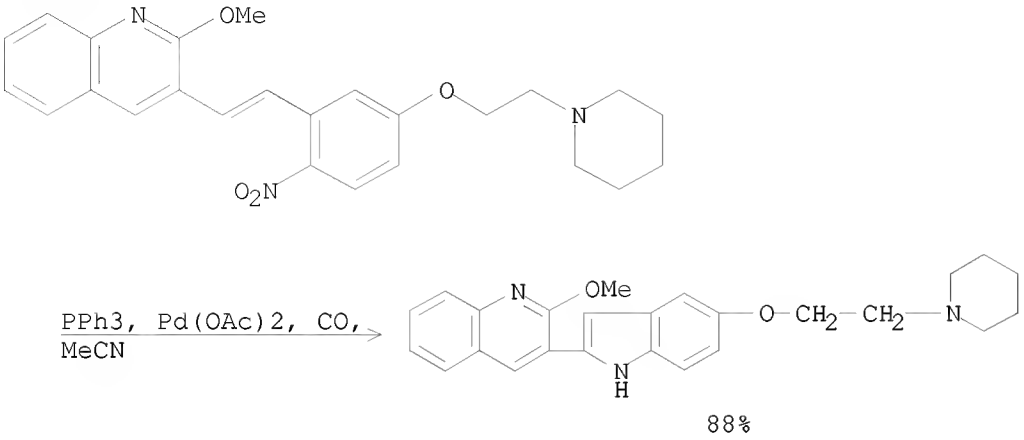
PPh3, Pd(OAc)2, CO,
MeCN



94%

NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

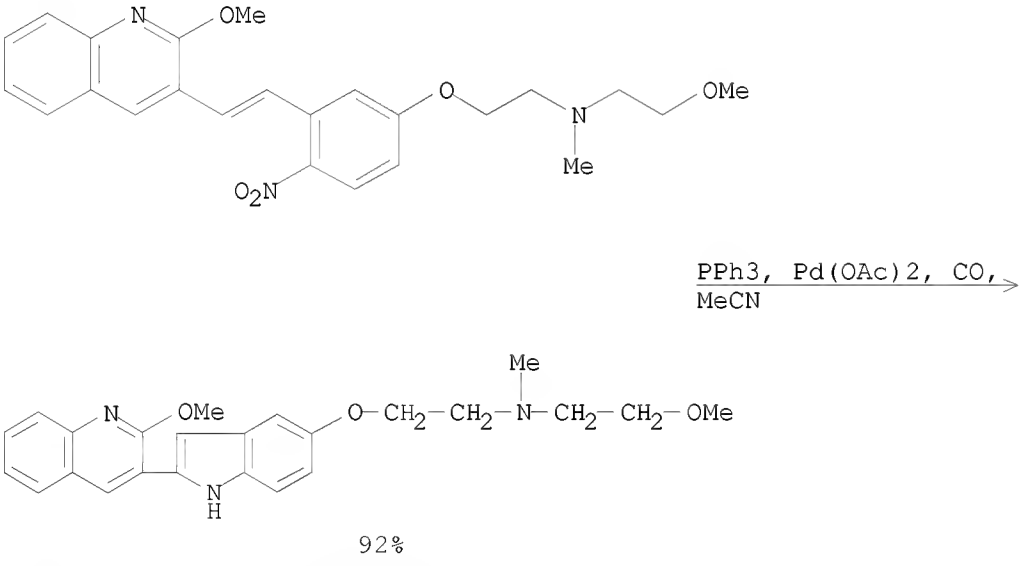
RX(10) OF 63



88%

NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

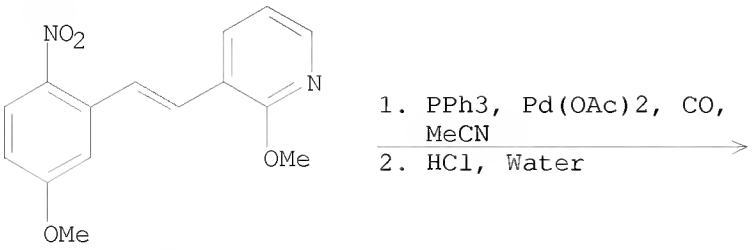
RX(15) OF 63



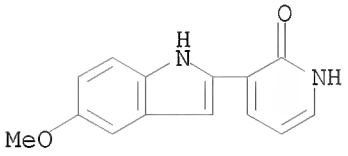
92%

NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

RX(17) OF 63



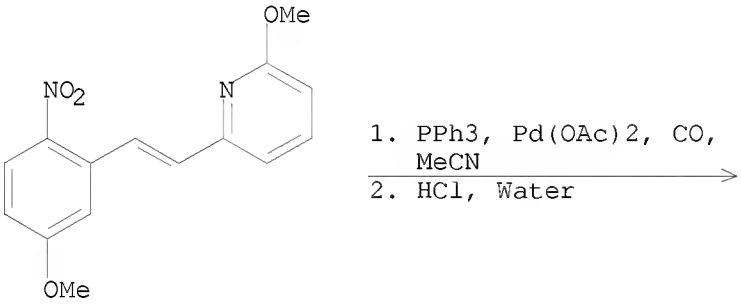
(step 1)



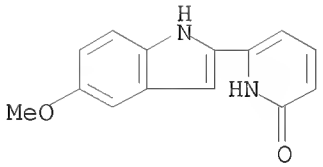
83%

CON: STAGE(1) 12 hours, 70 deg C, 6 atm
STAGE(2) 12 hours, reflux

RX(18) OF 63



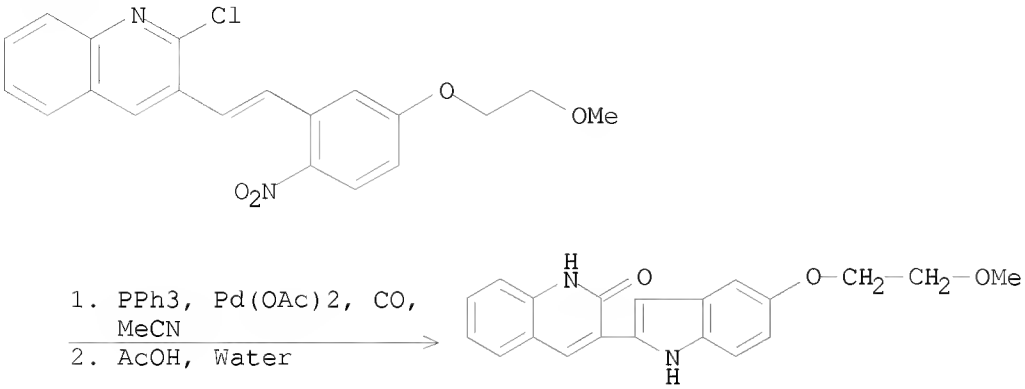
(step 1)



82%

CON: STAGE(1) 12 hours, 70 deg C, 6 atm
STAGE(2) 12 hours, reflux

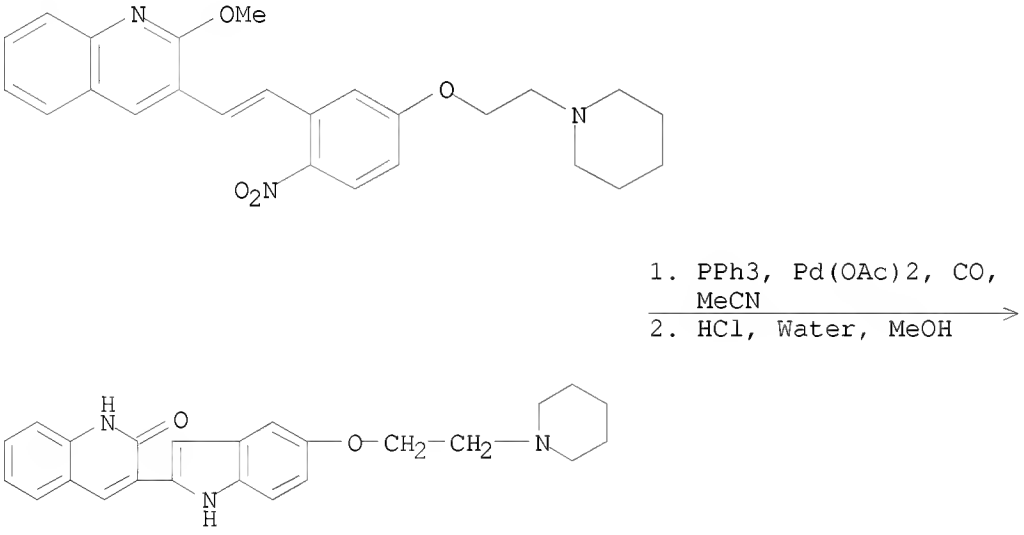
RX(25) OF 63 - 2 STEPS



98%

NOTE: 1) alternative prepn. shown, 2) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 3 hours, reflux

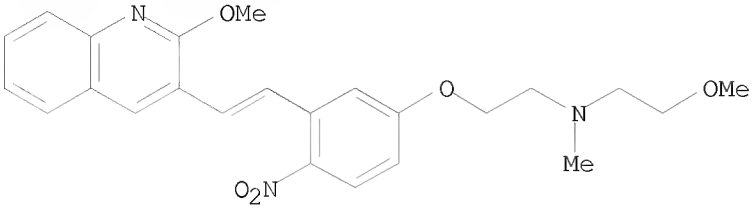
RX(29) OF 63 - 2 STEPS



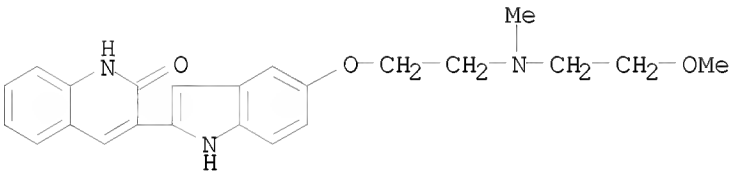
63%

NOTE: 1) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 4 hours, reflux

RX(33) OF 63 - 2 STEPS



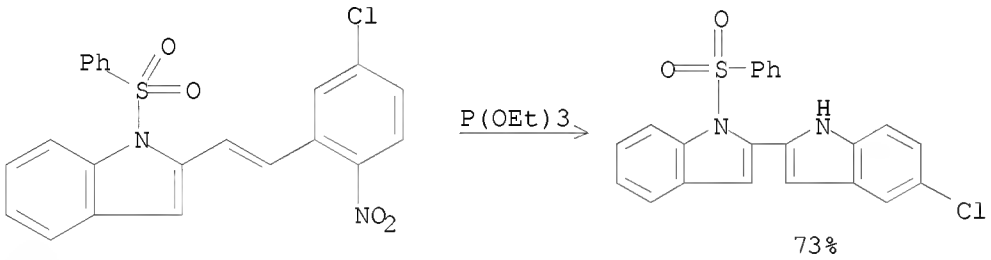
1. PPh3, Pd(OAc)2, CO, MeCN
2. HCl, Water, MeOH



NOTE: 1) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 4 hours, reflux

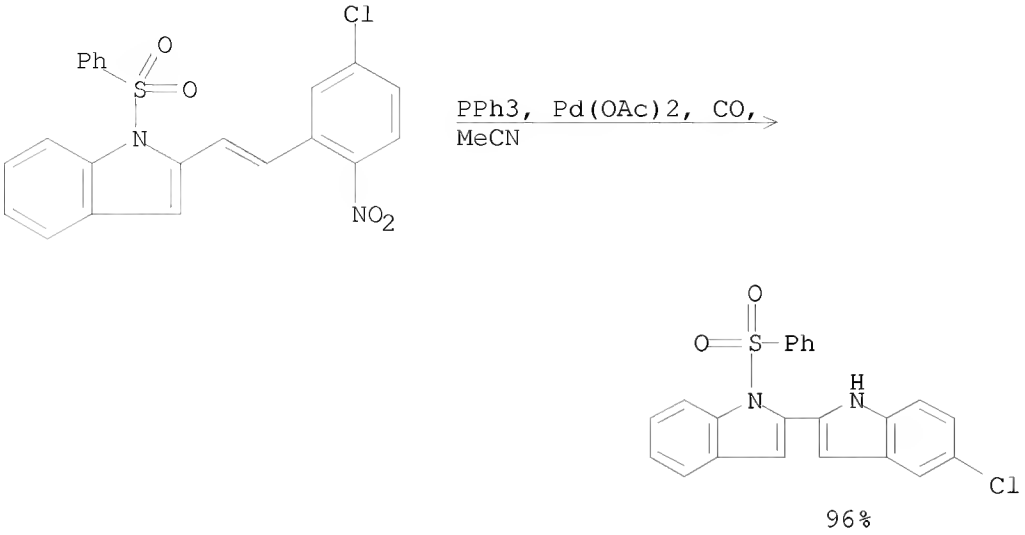
L4 ANSWER 10 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 71



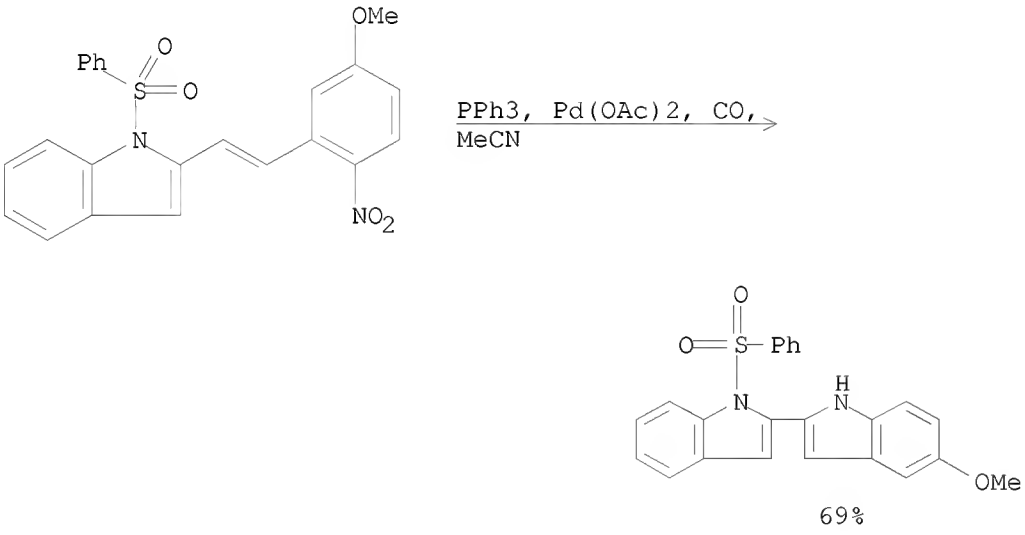
CON: 2 hours, 155 deg C

RX(4) OF 71



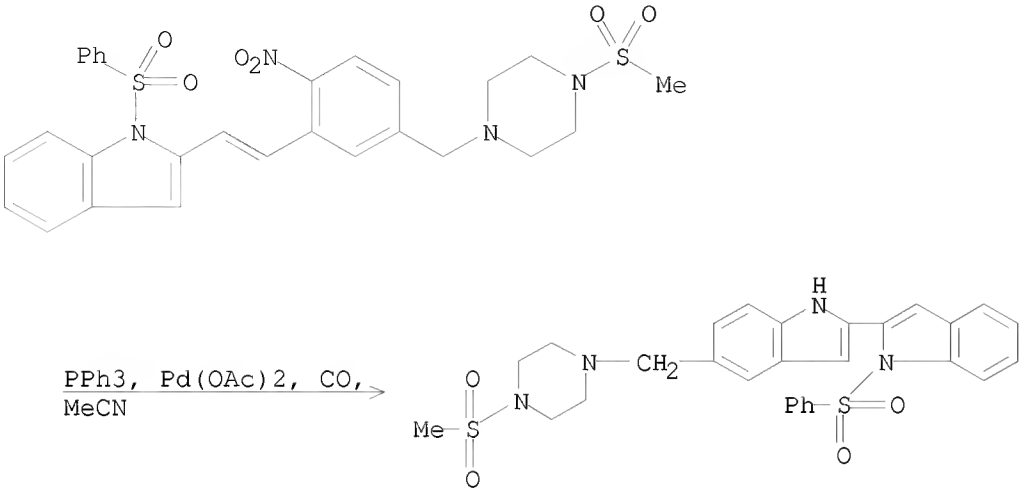
CON: 12 hours, 70 deg C

RX(6) OF 71



NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

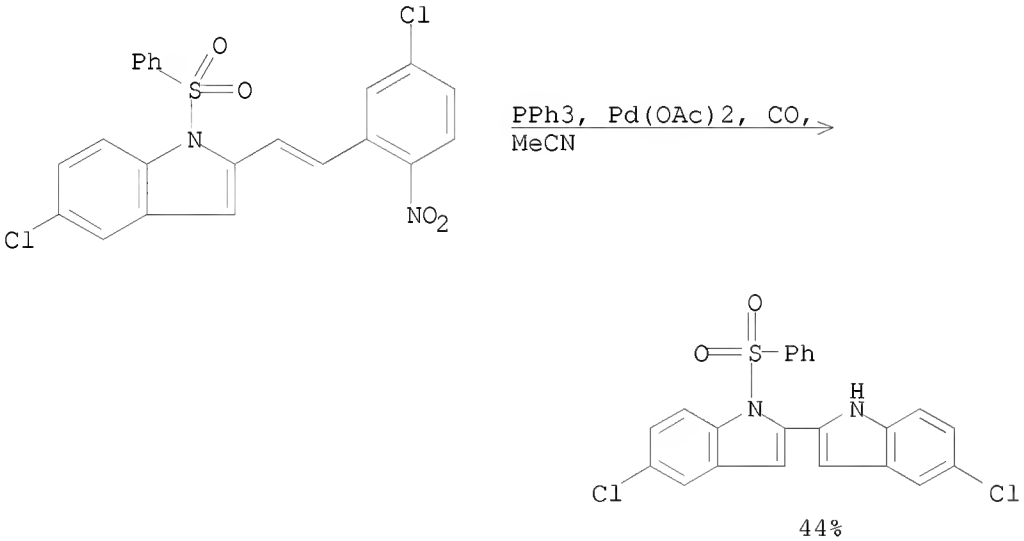
RX(7) OF 71



63%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

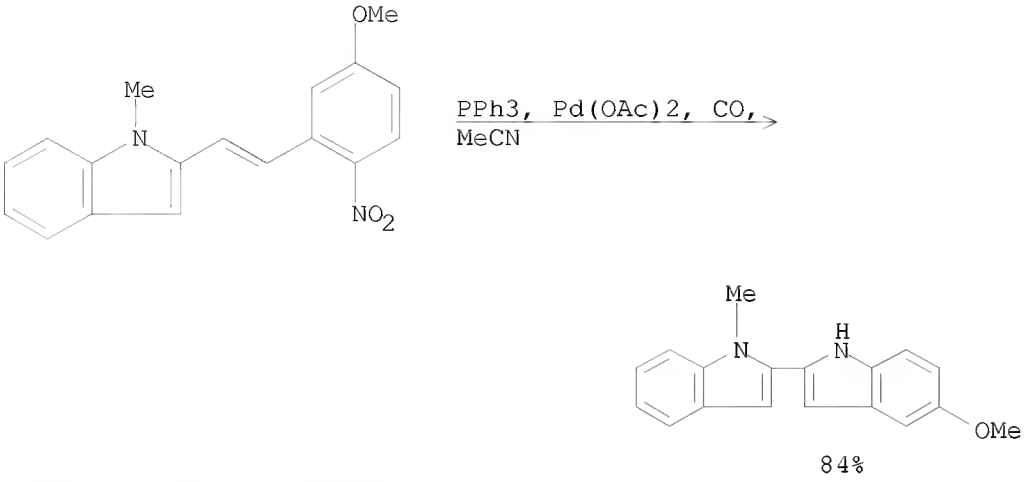
RX(9) OF 71



44%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

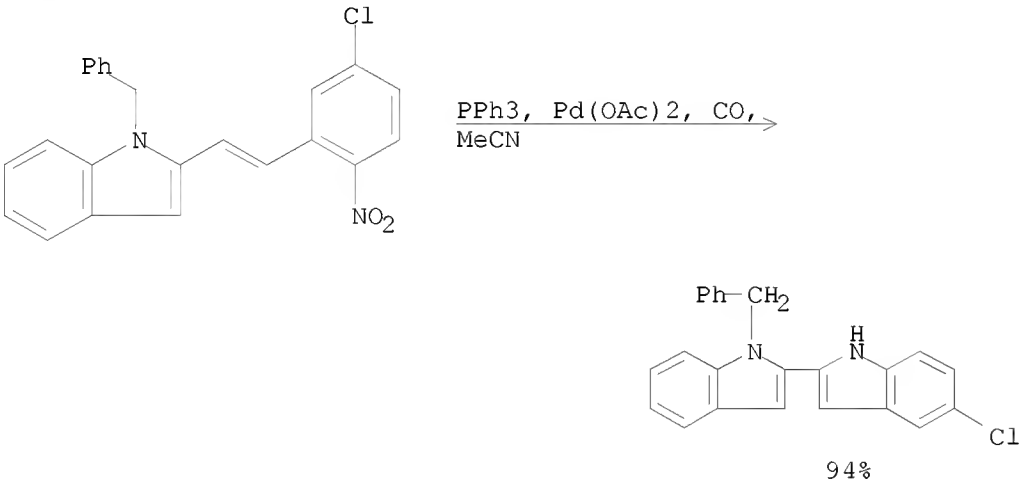
RX(11) OF 71



84%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

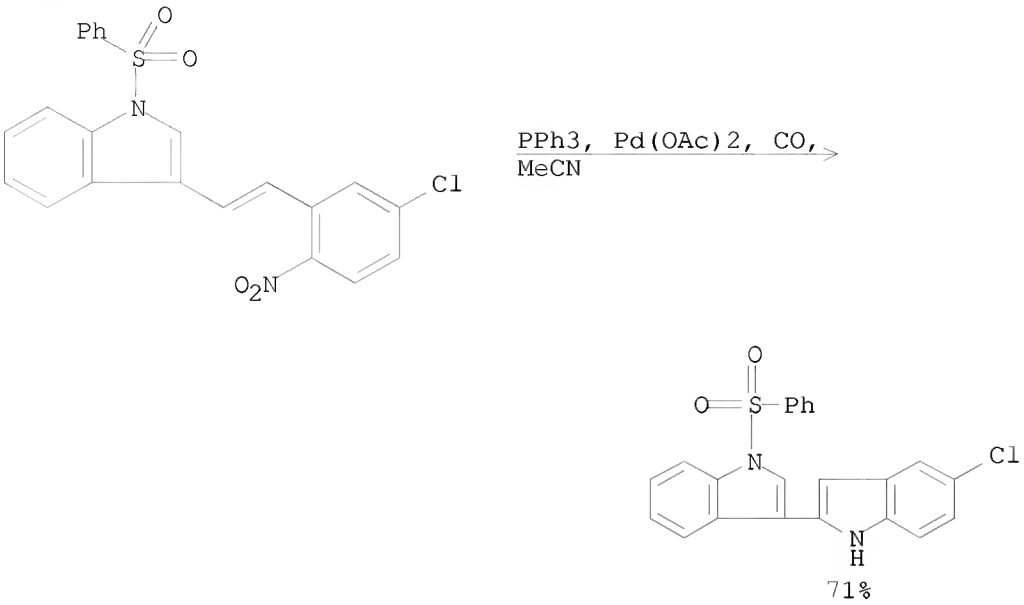
RX(14) OF 71



94%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

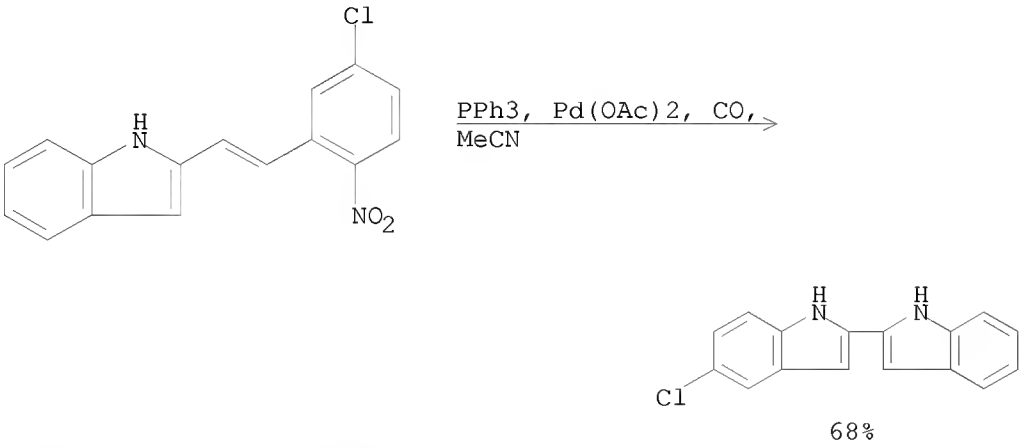
RX(16) OF 71



71%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

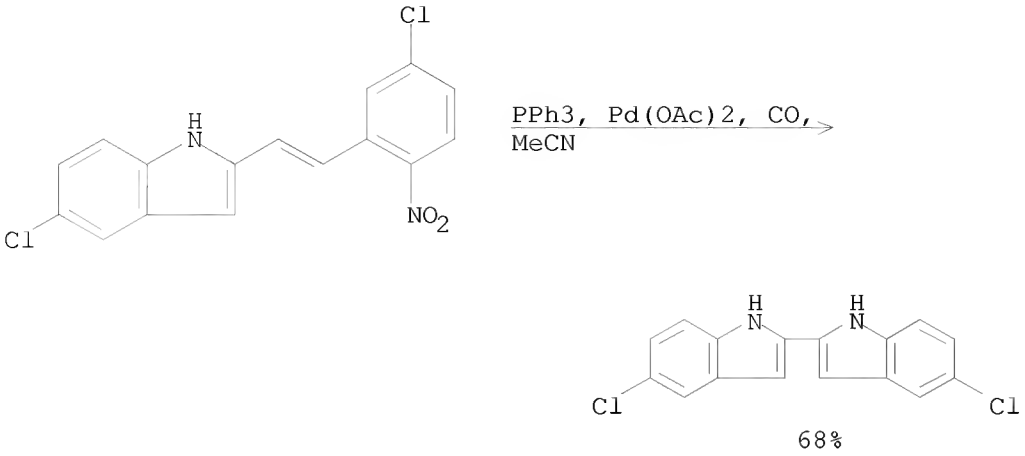
RX(18) OF 71



68%

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

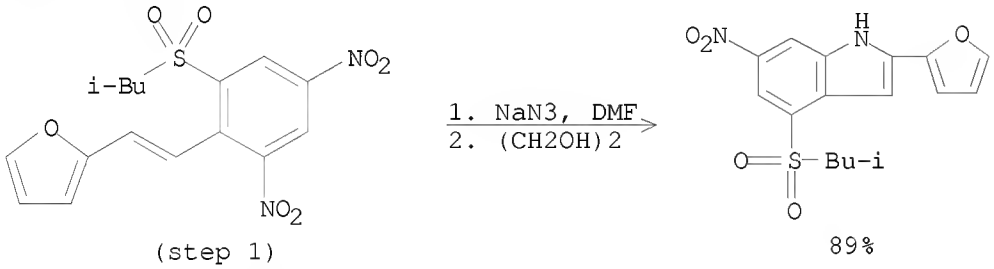
RX(21) OF 71



NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

L4 ANSWER 11 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(11) OF 29

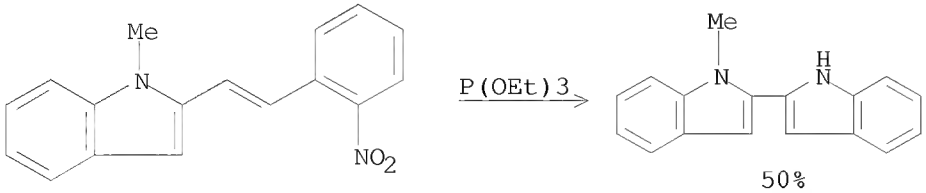


(step 1)

NOTE: regioselective, thermal, stereoselective

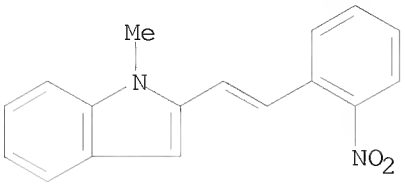
L4 ANSWER 12 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 177

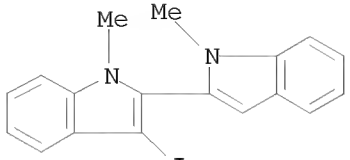


NOTE: thermal, alternative prepns. gave similar yields

RX(43) OF 177 - 2 STEPS



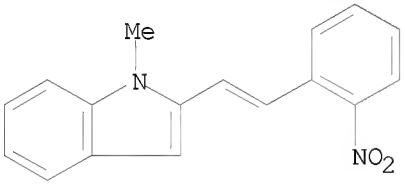
1. P(OEt)3
2.1. I2, KOH, DMF
2.2. MeI, NaH, DMF, Hexane



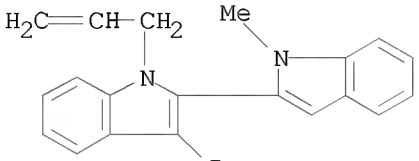
100%

NOTE: 1) thermal, alternative prepns. gave similar yields

RX(44) OF 177 - 2 STEPS



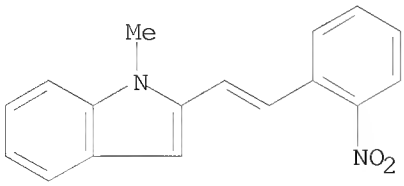
1. P(OEt)3
2.1. I2, KOH, DMF
2.2. Allyl bromide, NaH, DMF, Hexane



75%

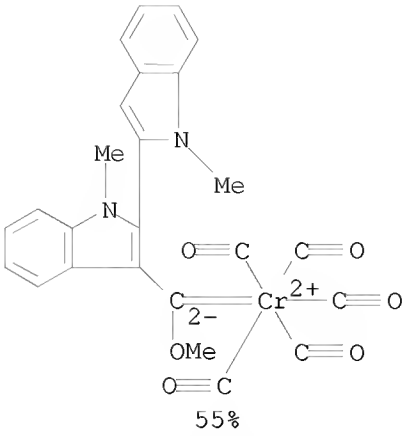
NOTE: 1) thermal, alternative prepns. gave similar yields, 2) reactant assumed

RX(79) OF 177 - 3 STEPS



1. P(OEt)3
2.1. I2, KOH, DMF
2.2. MeI, NaH, DMF, Hexane
3.1. BuLi, THF, Et2O
3.2. Cr(CO)6, Et2O
3.3. Na2CO3, Water
3.4. CF3SO3Me

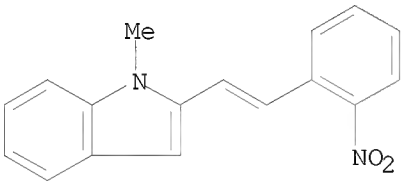
RX(79) OF 177 - 3 STEPS



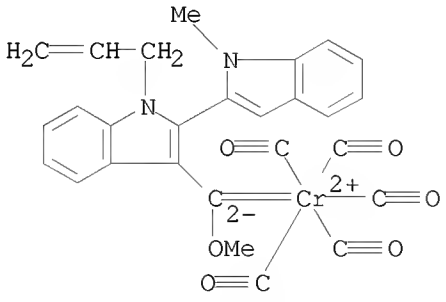
55%

NOTE: 1) thermal, alternative prepns. gave similar yields

RX(80) OF 177 - 3 STEPS



1. P(OEt)3
2.1. I2, KOH, DMF
2.2. Allyl bromide, NaH, DMF, Hexane
3.1. BuLi, THF, Et2O
3.2. Cr(CO)6, Et2O
3.3. Na2CO3, Water
3.4. CF3SO3Me

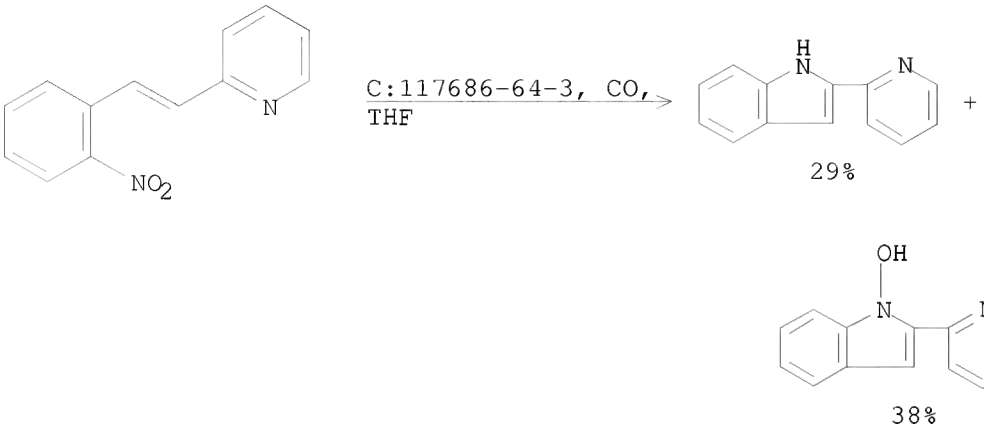


33%

NOTE: 1) thermal, alternative prepns. gave similar yields, 2) reactant assumed

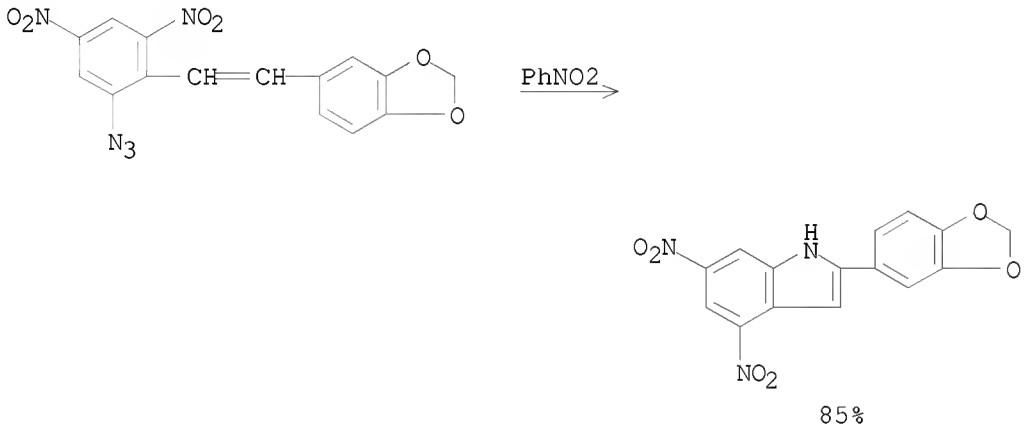
L4 ANSWER 13 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 5

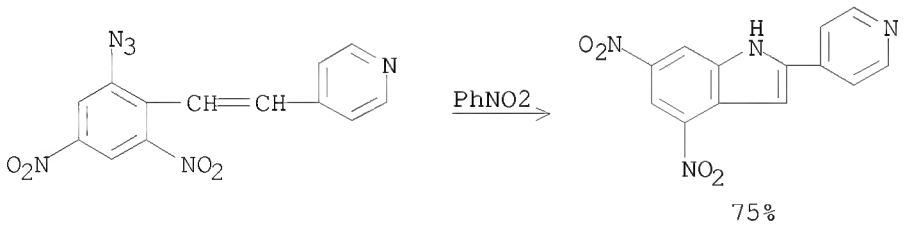


L4 ANSWER 14 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

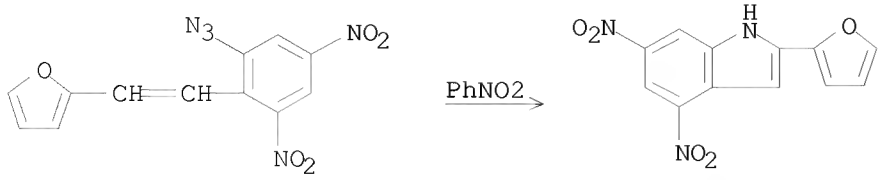
RX(22) OF 57



RX(24) OF 57

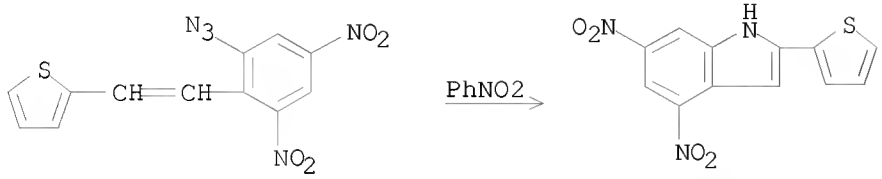


RX(25) OF 57



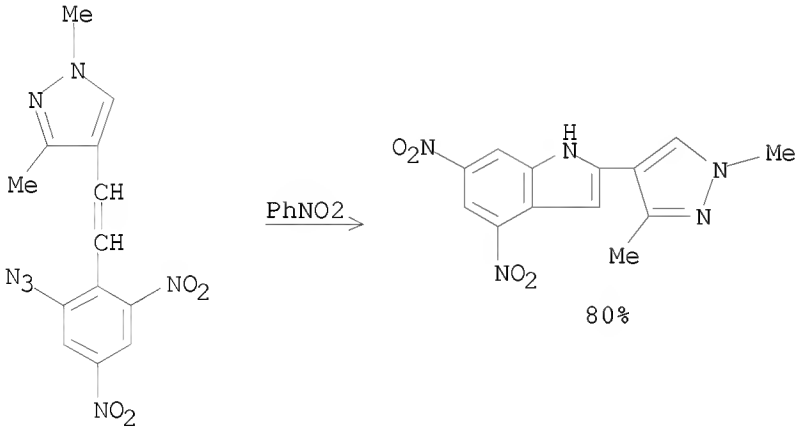
81%

RX(26) OF 57



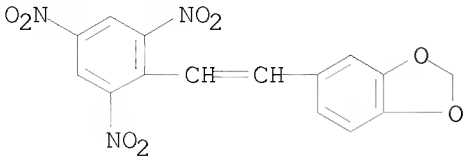
87%

RX(28) OF 57

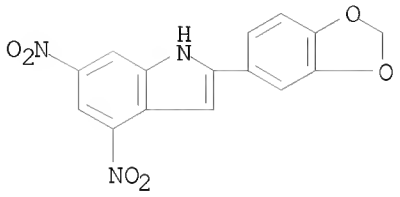


80%

RX(41) OF 57 - 2 STEPS

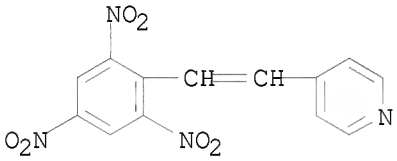


1.1. NaN3, DMF
1.2. Water
2. PhNO2

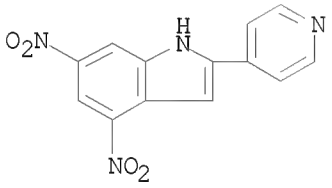


85%

RX(43) OF 57 - 2 STEPS

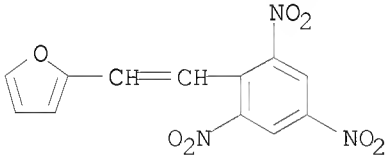


1.1. NaN3, DMF
1.2. Water
2. PhNO2

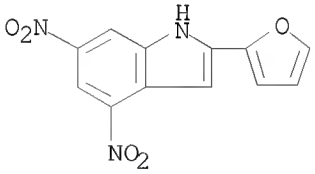


75%

RX(44) OF 57 - 2 STEPS

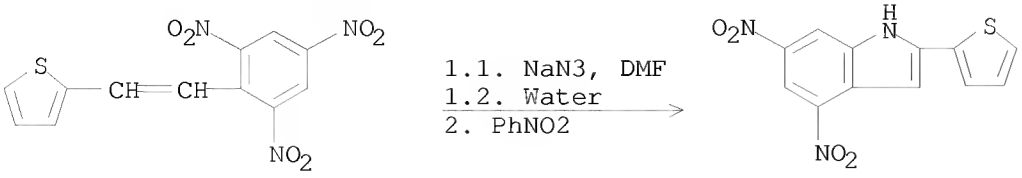


1.1. NaN3, DMF
1.2. Water
2. PhNO2



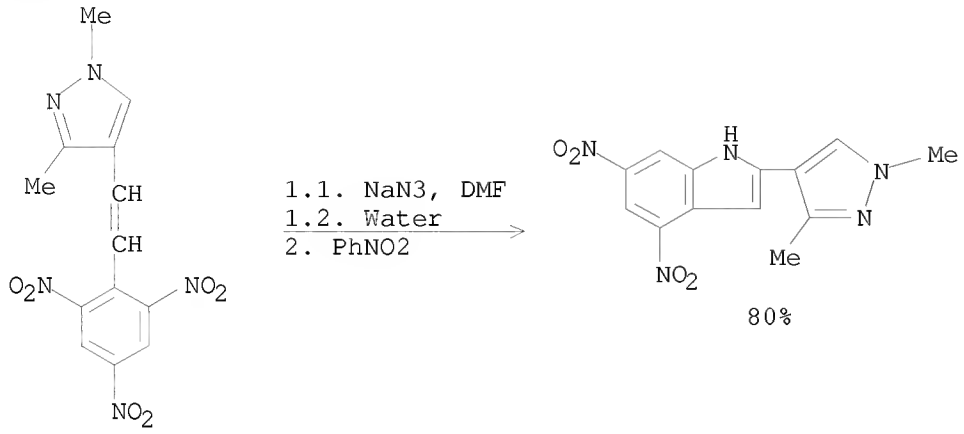
81%

RX(45) OF 57 - 2 STEPS



87%

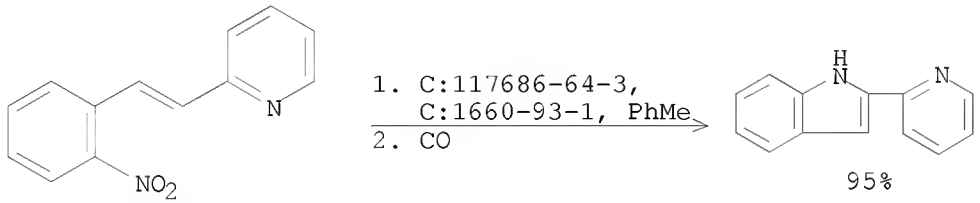
RX(47) OF 57 - 2 STEPS



80%

L4 ANSWER 15 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

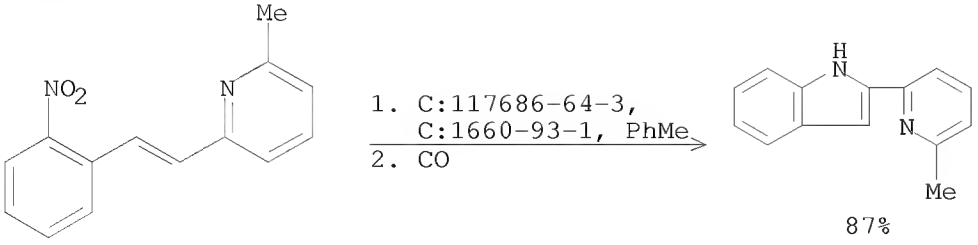
RX(1) OF 9



(step 1)

95%

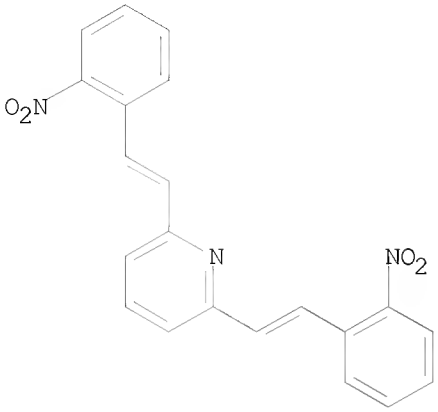
RX(2) OF 9



(step 1)

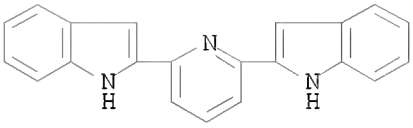
87%

RX(3) OF 9



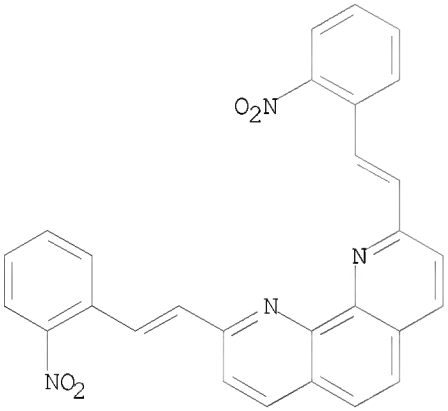
(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



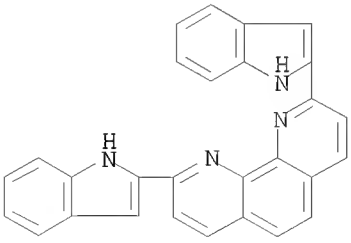
56%

RX(4) OF 9



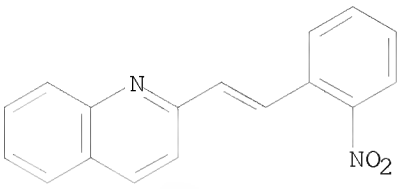
(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



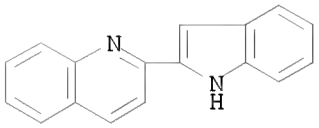
65%

RX(5) OF 9



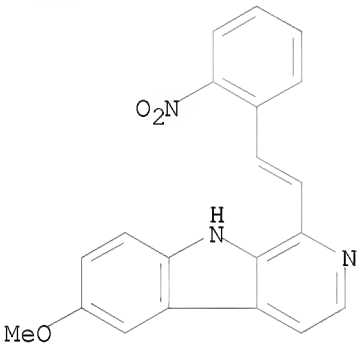
1. C:117686-64-3,
   C:1660-93-1, PhMe
2. CO

(step 1)



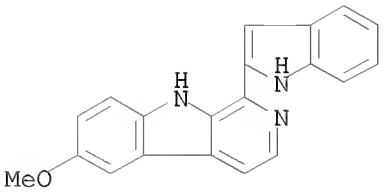
76%

RX(6) OF 9



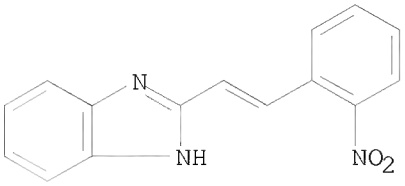
1. C:117686-64-3,
   C:1660-93-1, PhMe
2. CO

(step 1)



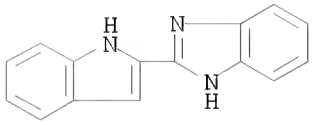
58%

RX(7) OF 9



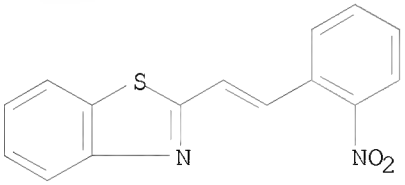
(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



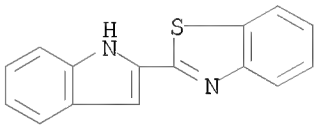
81%

RX(8) OF 9



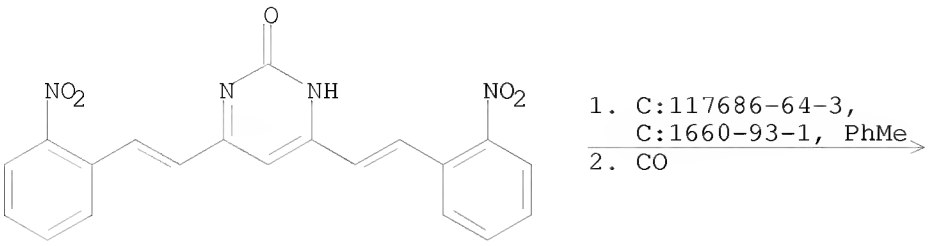
(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



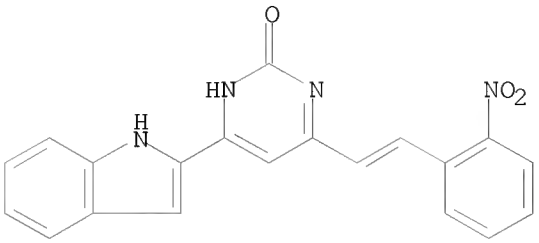
83%

RX(9) OF 9



1. C:117686-64-3, C:1660-93-1, PhMe
2. CO

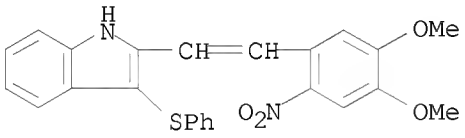
(step 1)



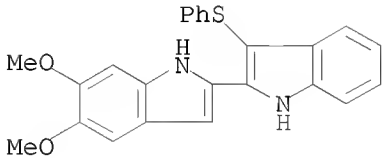
75%

L4 ANSWER 16 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

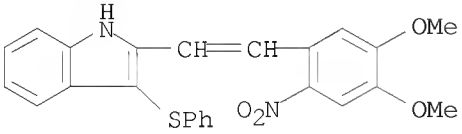
RX(2) OF 6



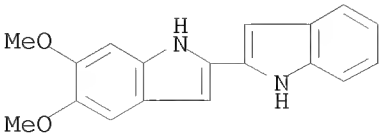
P(OEt)3



RX(5) OF 6 - 2 STEPS

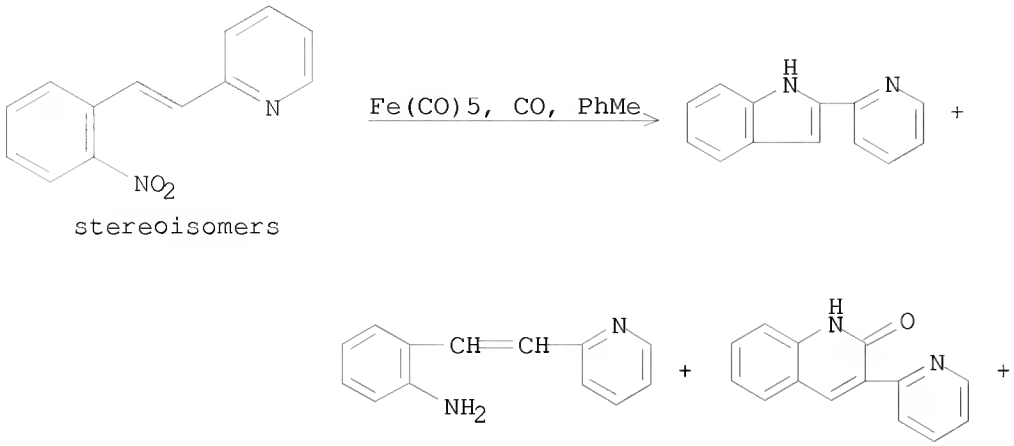


1. P(OEt)3
2. Ni, EtOH

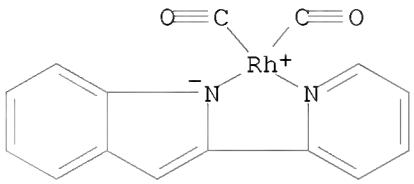


L4 ANSWER 17 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

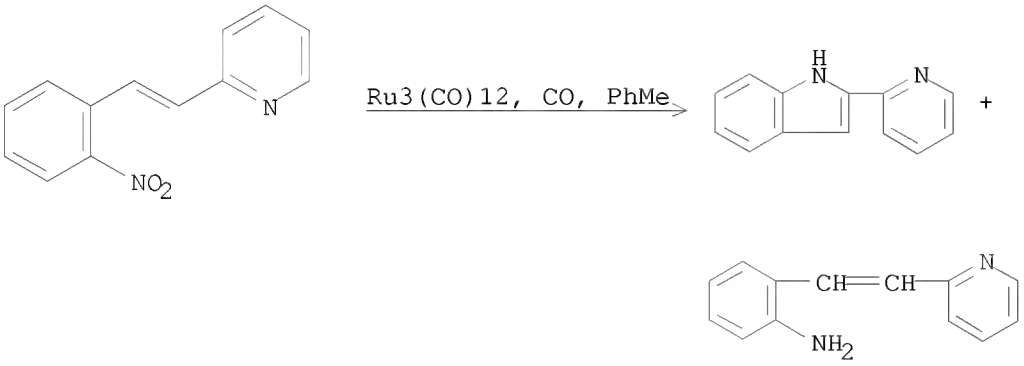
RX(8) OF 12



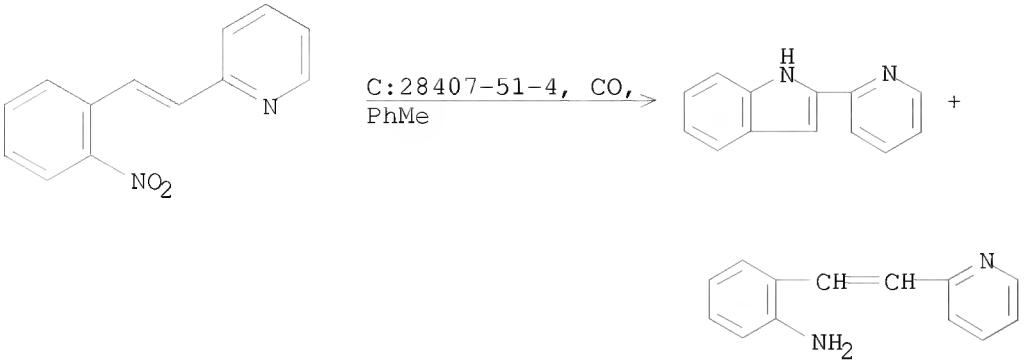
RX(8) OF 12



RX(9) OF 12

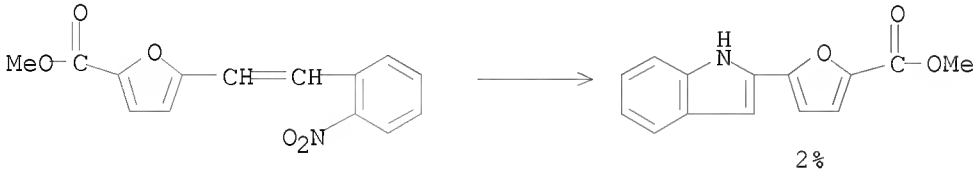


RX(10) OF 12

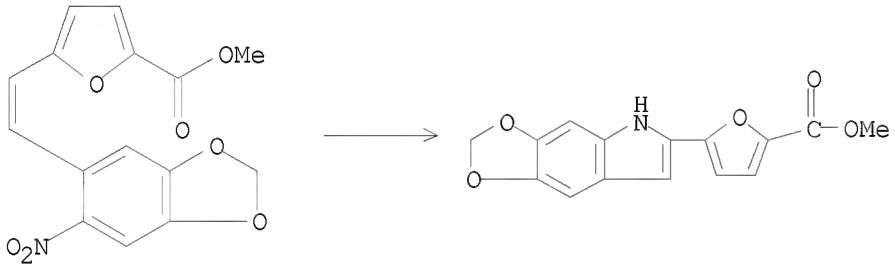


L4 ANSWER 18 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

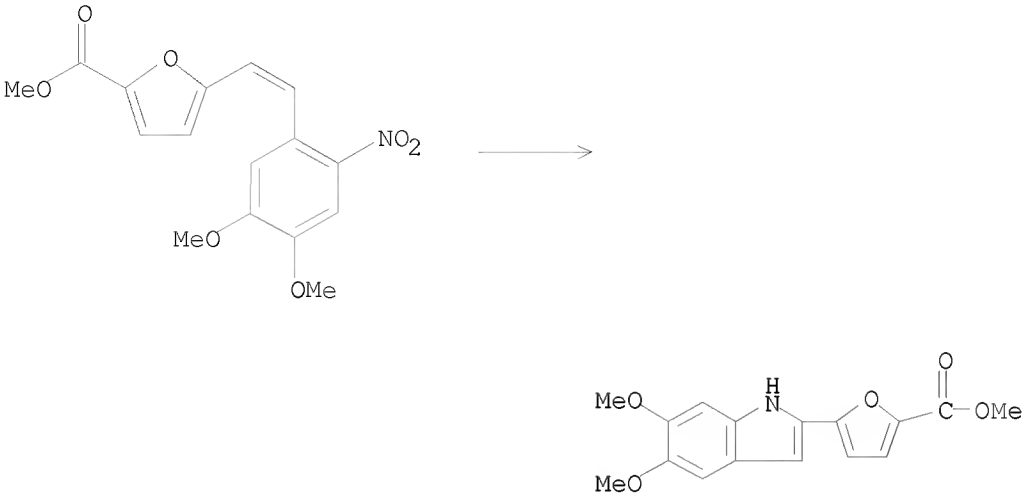
RX(69) OF 98 - 3 STEPS



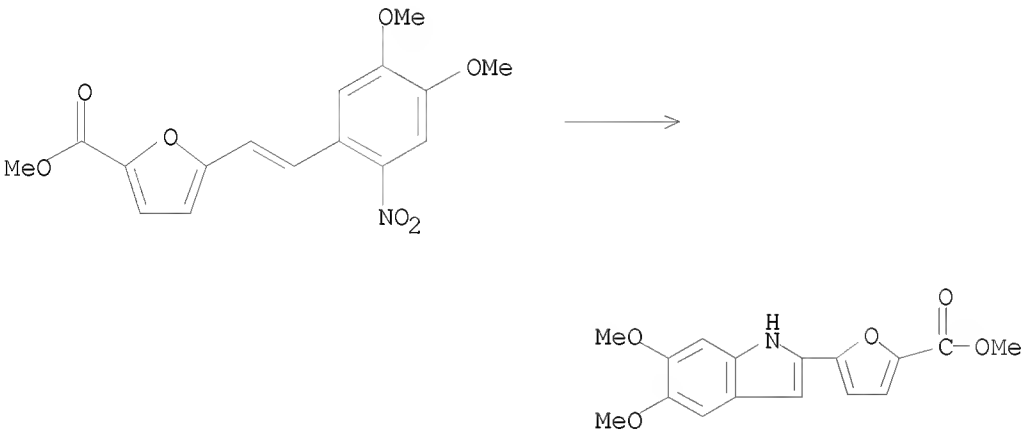
RX(72) OF 98 - 3 STEPS



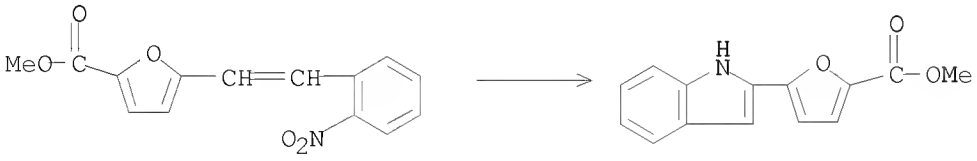
RX(73) OF 98 - 3 STEPS



RX(76) OF 98 - 3 STEPS



RX(80) OF 98 - 4 STEPS



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=> d 1-18 crdef abs
'CRDEF' IS NOT A VALID FORMAT FOR FILE 'CASREACT'
```

The following are valid formats:

```
ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
```

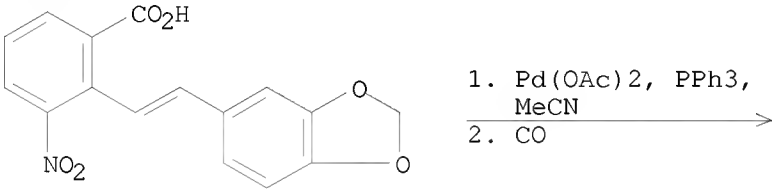
contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

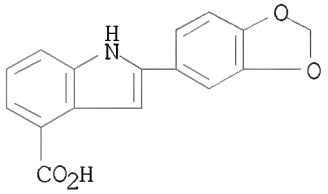
ENTER DISPLAY FORMAT (FCRDREF):crdref

L4 ANSWER 1 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(15) OF 47



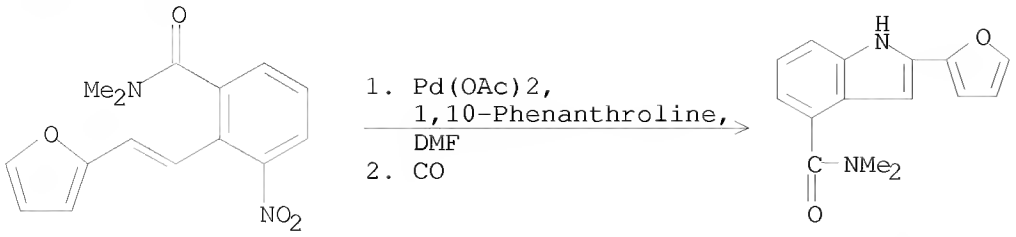
(step 1)



92%

REF: Tetrahedron, 62(49), 11381-11390; 2006
CON: STAGE(1) room temperature -> 70 deg C
STAGE(2) 16 hours, 70 deg C, 60 psi

RX(23) OF 47

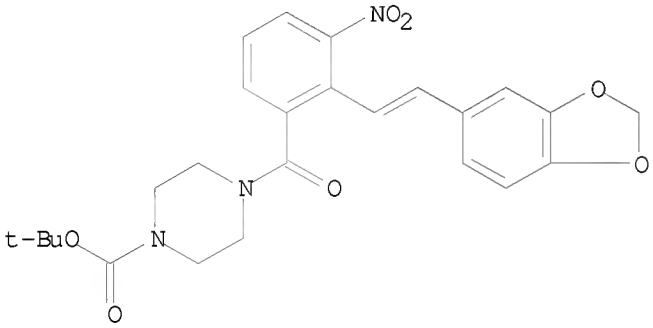


(step 1)

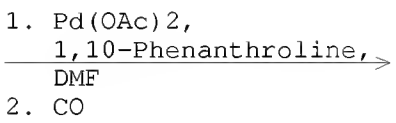
98%

REF: Tetrahedron, 62(49), 11381-11390; 2006
CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

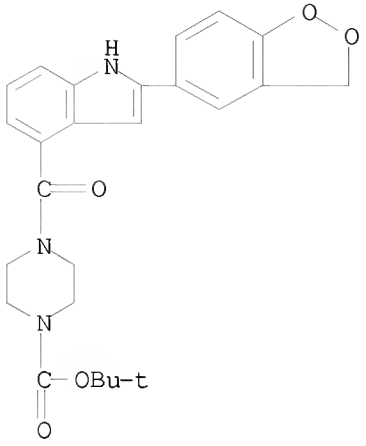
RX(25) OF 47



(step 1)



RX(25) OF 47



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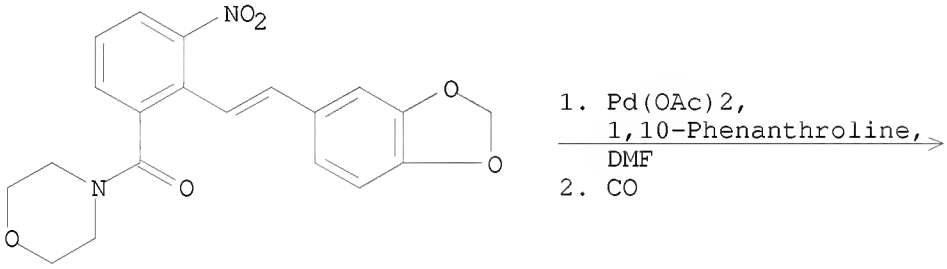
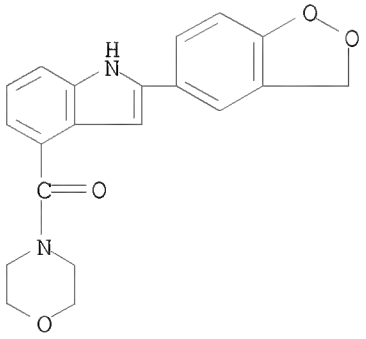
REF: Tetrahedron, 62(49), 11381-11390; 2006
CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(27) OF 47



(step 1)



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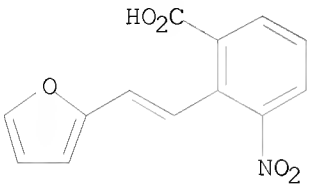
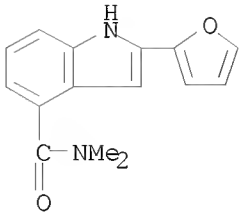
REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STAGE(1) room temperature -> 80 deg C
STAGE(2) 16 hours, 80 deg C, 30 psi

RX(37) OF 47 - 2 STEPS



1.1. DMF, (COCl)2, CH2Cl2
1.2. Me2NH, Et3N, CH2Cl2
2.1. Pd(OAc)2, 1,10-Phenanthroline, DMF
2.2. CO



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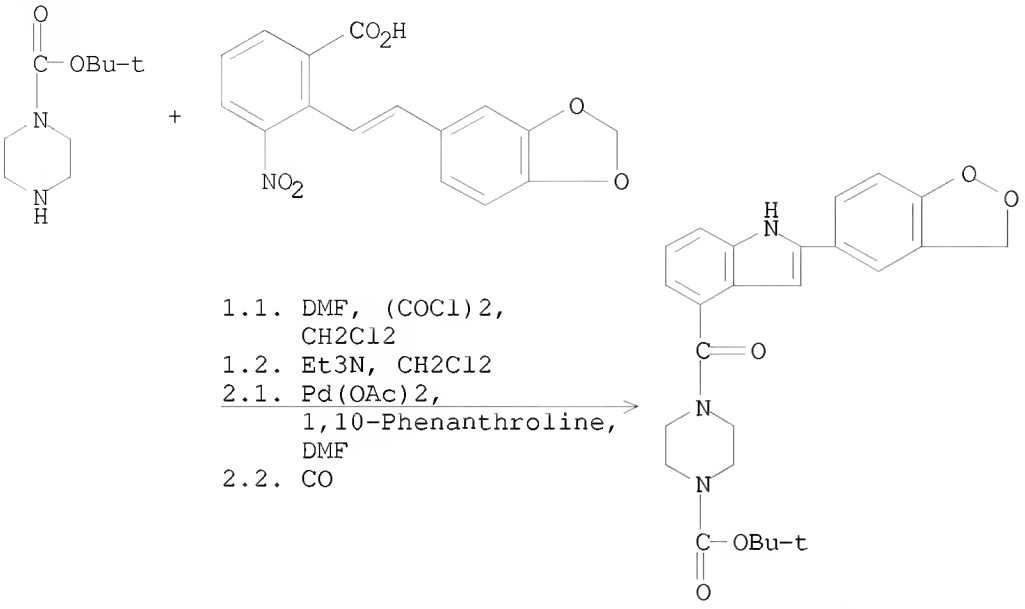
REF: Tetrahedron, 62(49), 11381-11390; 2006
CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(39) OF 47 - 2 STEPS



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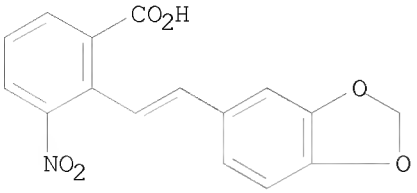
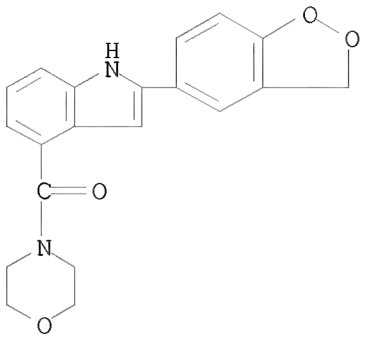
REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

RX(41) OF 47 - 2 STEPS



1.1. DMF, (COCl)2, CH2Cl2
1.2. Morpholine, Et3N, CH2Cl2
2.1. Pd(OAc)2, 1,10-Phenanthroline, DMF
2.2. CO



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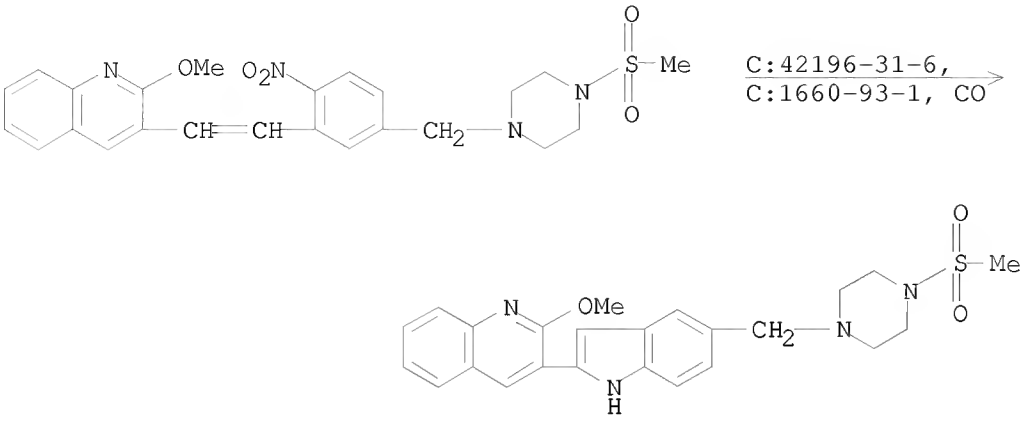
REF: Tetrahedron, 62(49), 11381-11390; 2006

CON: STEP(1.1) 1.5 hours, room temperature
STEP(1.2) room temperature; 30 minutes, room temperature
STEP(2.1) room temperature -> 80 deg C
STEP(2.2) 16 hours, 80 deg C, 30 psi

L4 ANSWER 2 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

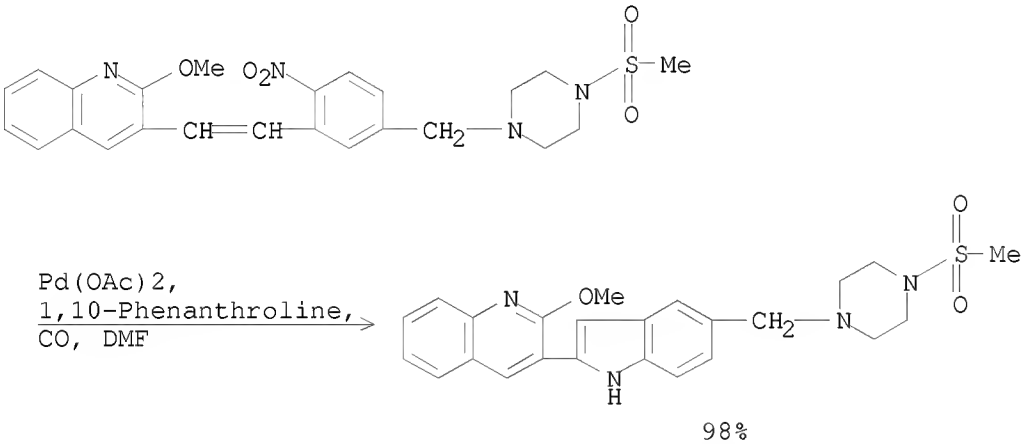
RX(2) OF 2



REF: JALA, 10(6), 394-407; 2005
NOTE: optimization study, optimized on catalyst loading, optimized on pressure, optimized on temperature
CON: 70 - 80 deg C, 15 psi

L4 ANSWER 3 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 47



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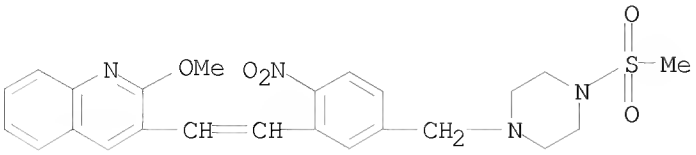
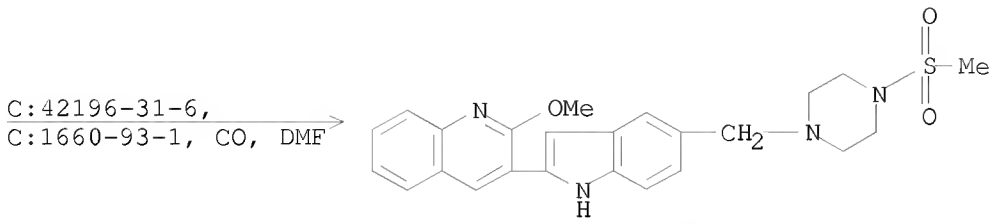
REF: Tetrahedron, 61(26), 6425-6437; 2005
NOTE: optimization study, green chem. - waste reduction
CON: 70 deg C, 15 psi

RX(2) OF 47





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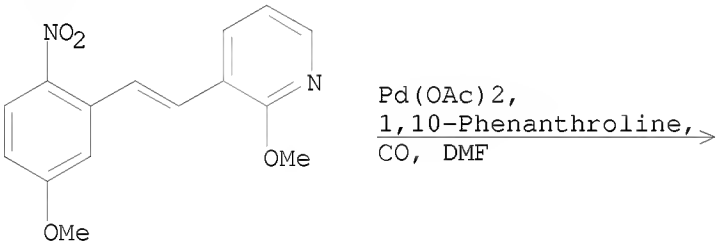
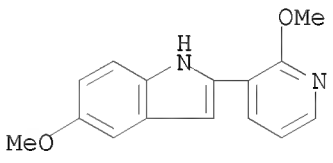
REF: Tetrahedron, 61(26), 6425-6437; 2005
NOTE: optimization study, green chem. - waste reduction
CON: 70 deg C, 15 psi

RX(23) OF 47

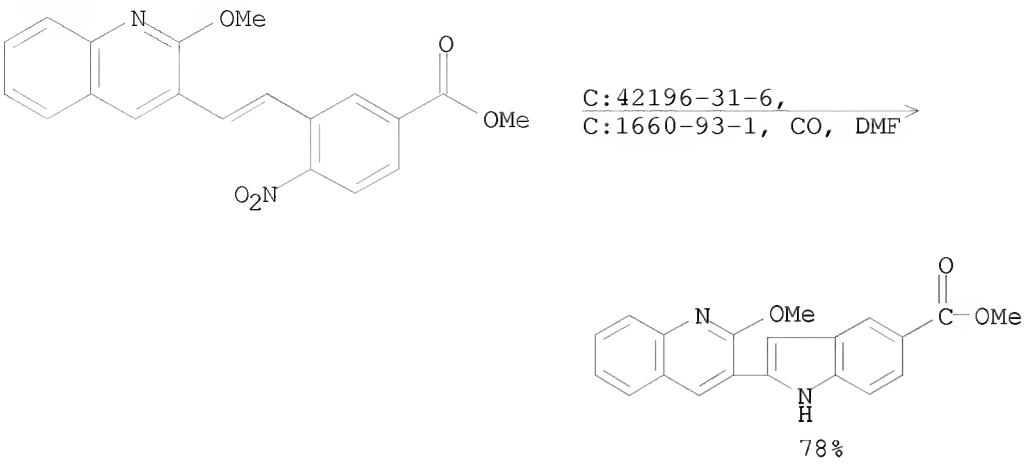




72%

REF: Tetrahedron, 61(26), 6425-6437; 2005
NOTE: green chem. - waste reduction
CON: 16 hours, 70 deg C, 30 psi

RX(24) OF 47



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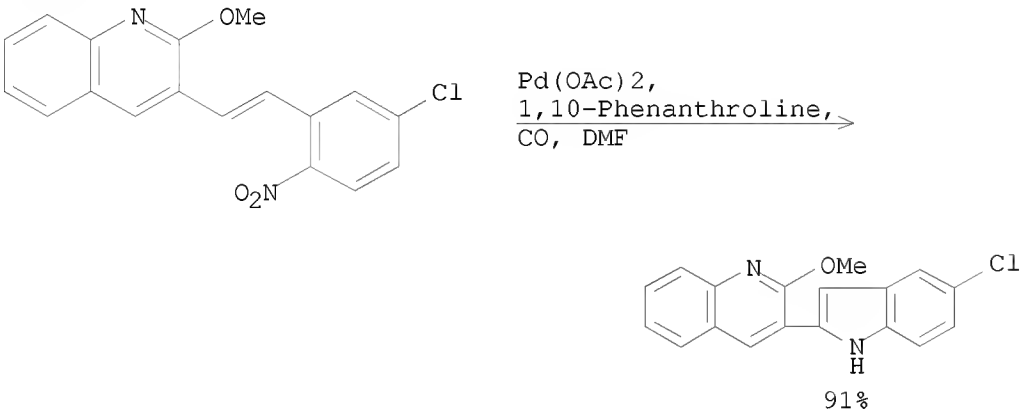
REF: Tetrahedron, 61(26), 6425-6437; 2005
NOTE: green chem. - waste reduction
CON: 16 hours, 80 deg C, 15 psi

RX(25) OF 47



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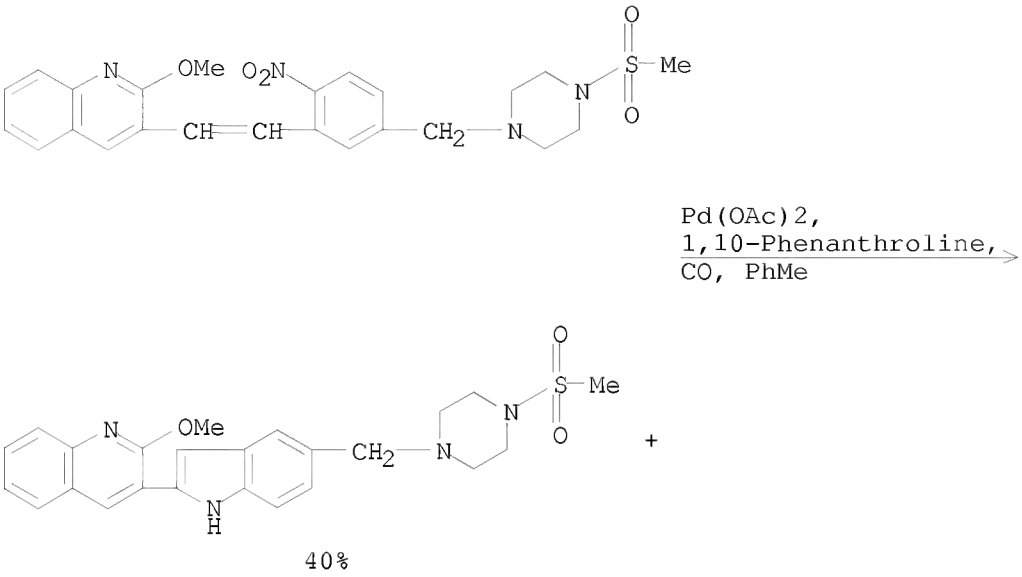
REF: Tetrahedron, 61(26), 6425-6437; 2005
NOTE: green chem. - waste reduction
CON: 16 hours, 80 deg C, 15 psi

RX(28) OF 47



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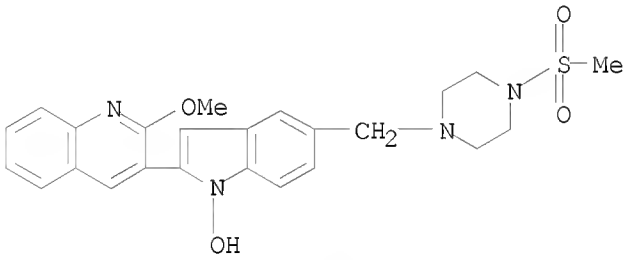
RX(28) OF 47



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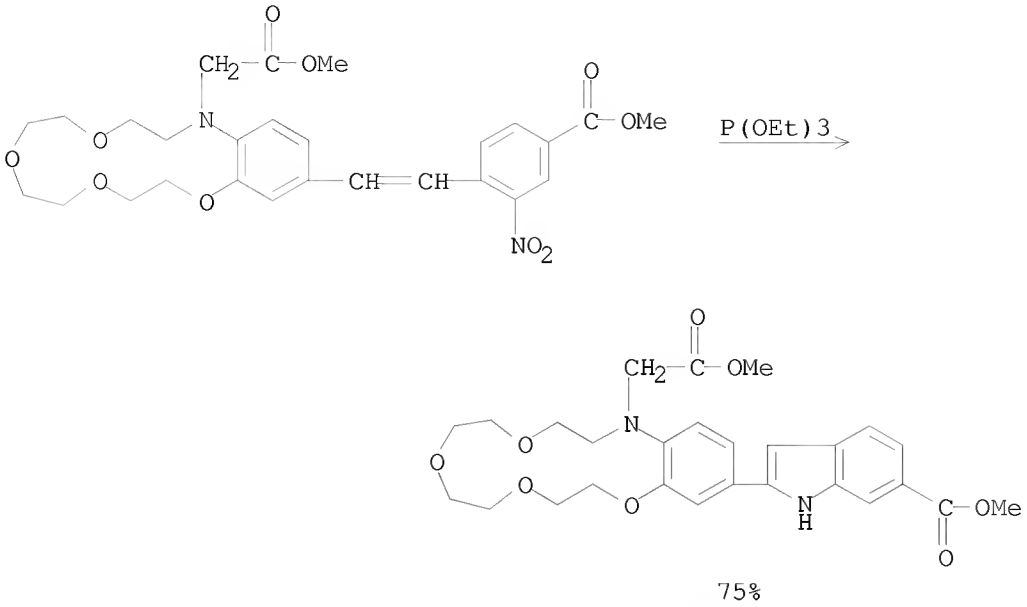
REF: Tetrahedron, 61(26), 6425-6437; 2005
CON: 70 deg C, 15 psi

L4 ANSWER 4 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(28) OF 161



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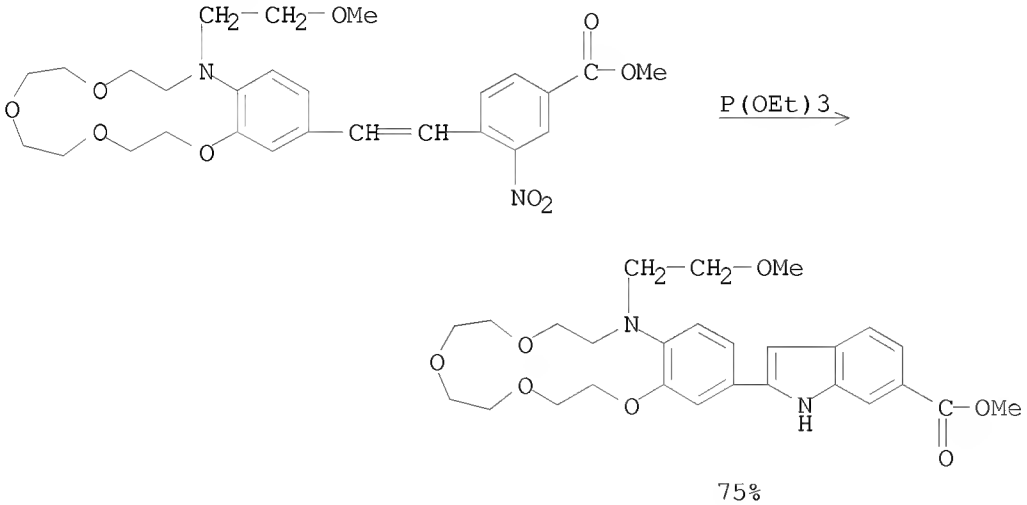
REF: Bioorganic & Medicinal Chemistry Letters, 15(7), 1851-1855; 2005

RX(29) OF 161



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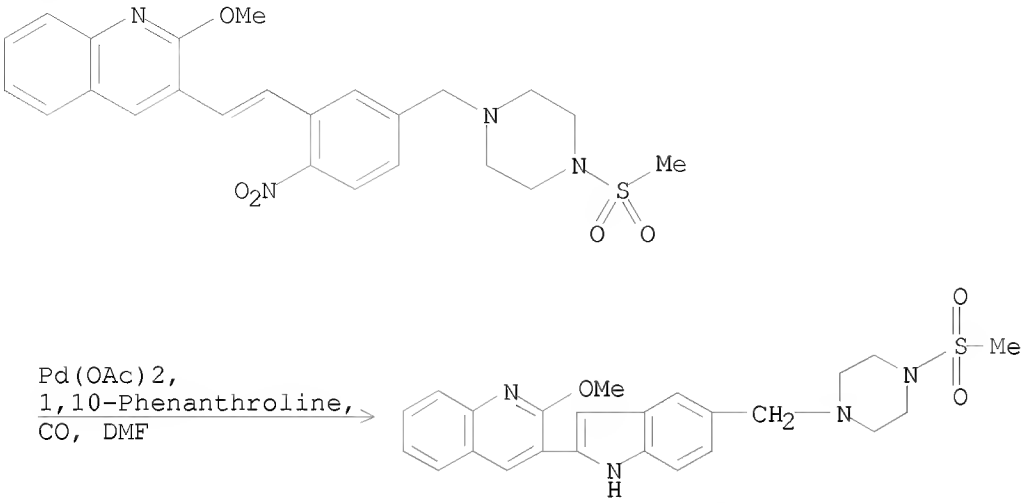
REF: Bioorganic & Medicinal Chemistry Letters, 15(7), 1851-1855; 2005

L4 ANSWER 5 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

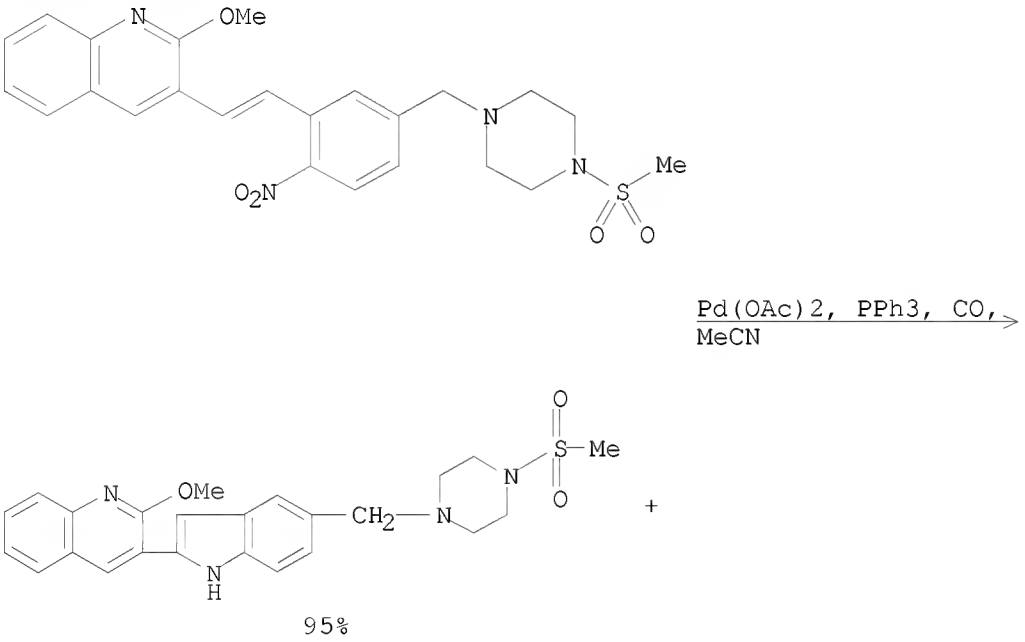
RX(36) OF 350



94%

REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005
CON: 14 hours, 70 deg C, 15 psi

RX(37) OF 350



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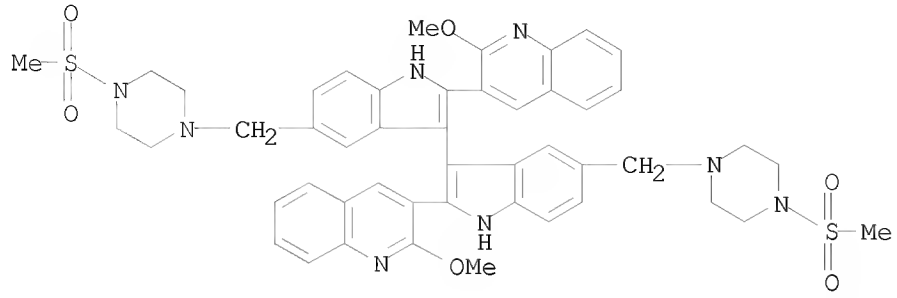
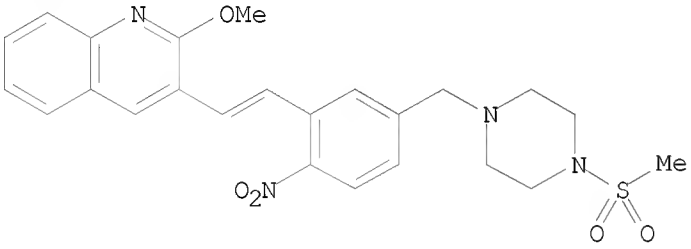
RX(37) OF 350



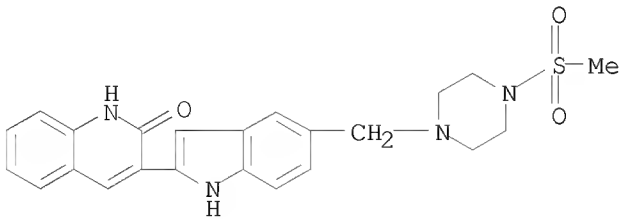
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005
CON: 15 hours, 70 deg C, 60 atm

RX(59) OF 350 - 2 STEPS



1. Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF
2. HCl, Water, DMF

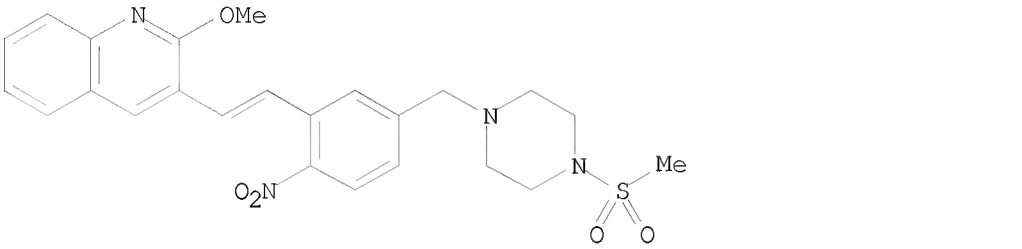
RX(59) OF 350 - 2 STEPS



HCl
100%

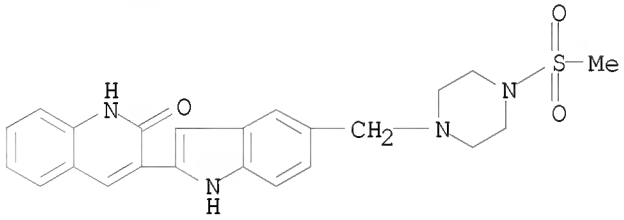
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005
CON: STEP(1) 14 hours, 70 deg C, 15 psi

RX(60) OF 350 - 2 STEPS



1. Pd(OAc)2, PPh3, CO, MeCN
2. HCl, Water, DMF

RX(60) OF 350 - 2 STEPS

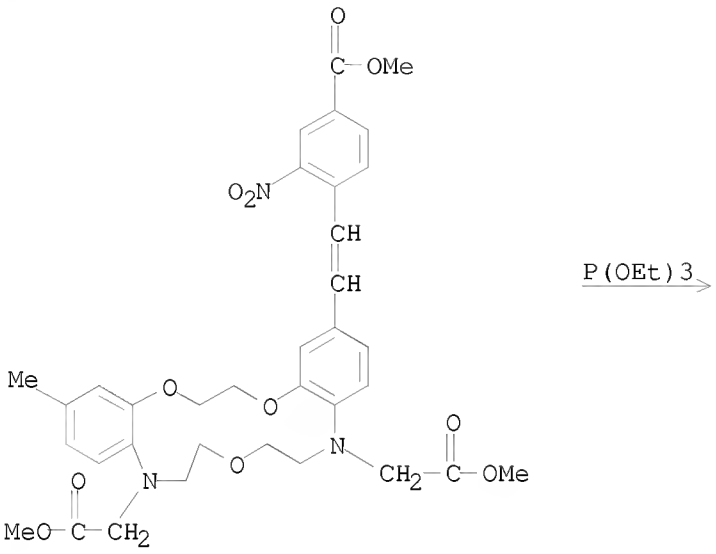


HCl
100%

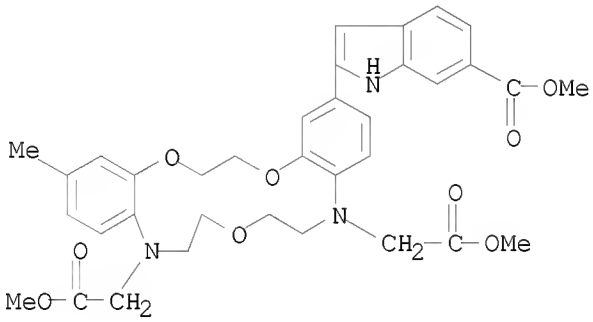
REF: Journal of Organic Chemistry, 70(7), 2555-2567; 2005
CON: STEP(1) 15 hours, 70 deg C, 60 atm

L4 ANSWER 6 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(26) OF 555



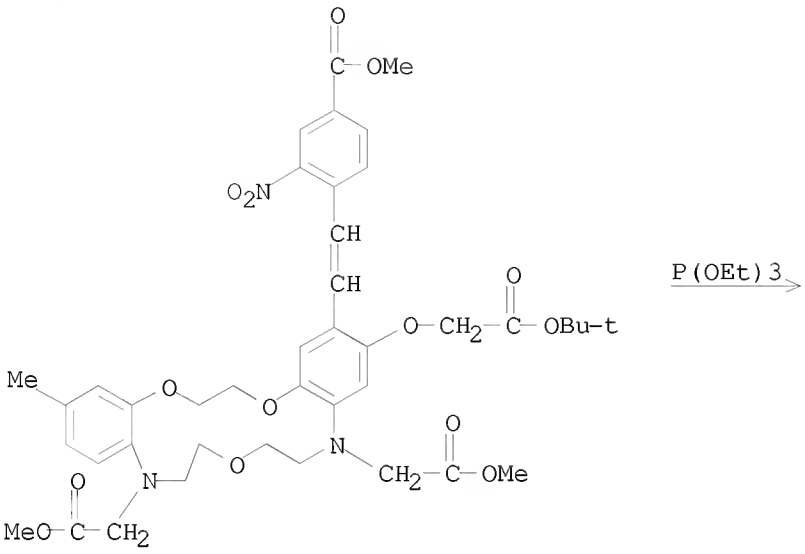
RX(26) OF 555



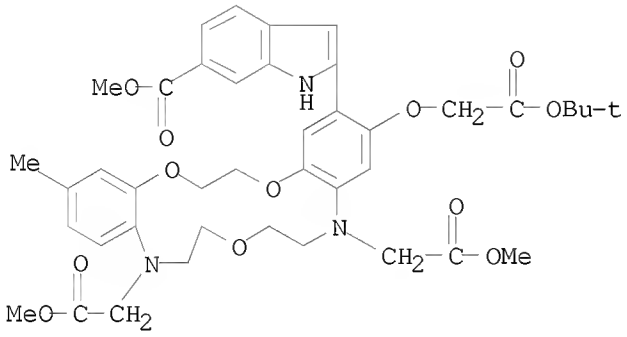
80%

REF: PCT Int. Appl., 2005016874, 24 Feb 2005
CON: 6 hours, 120 deg C

RX(48) OF 555



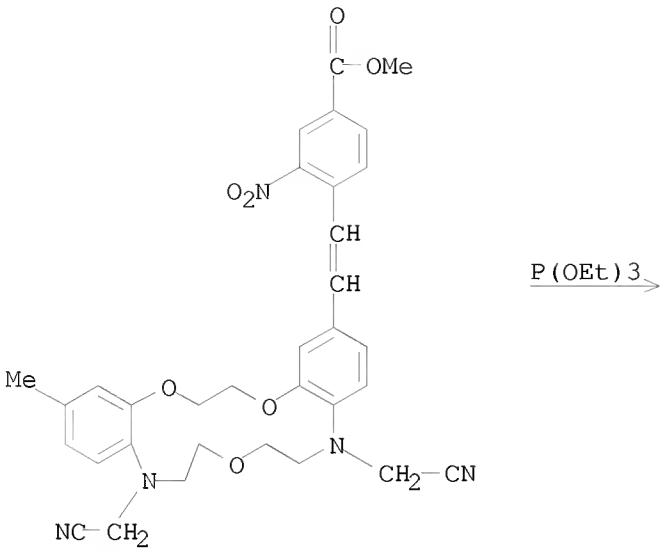
RX(48) OF 555



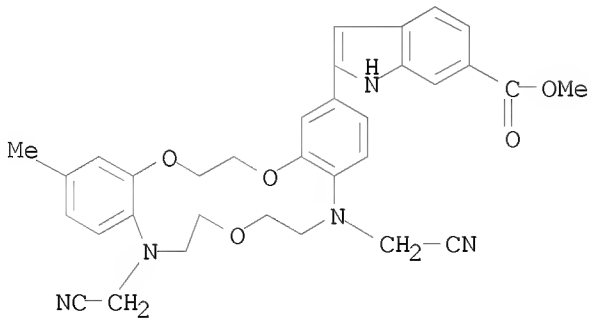
34%

REF: PCT Int. Appl., 136 pp.; 2005
CON: 7 hours, 130 deg C

RX(54) OF 555



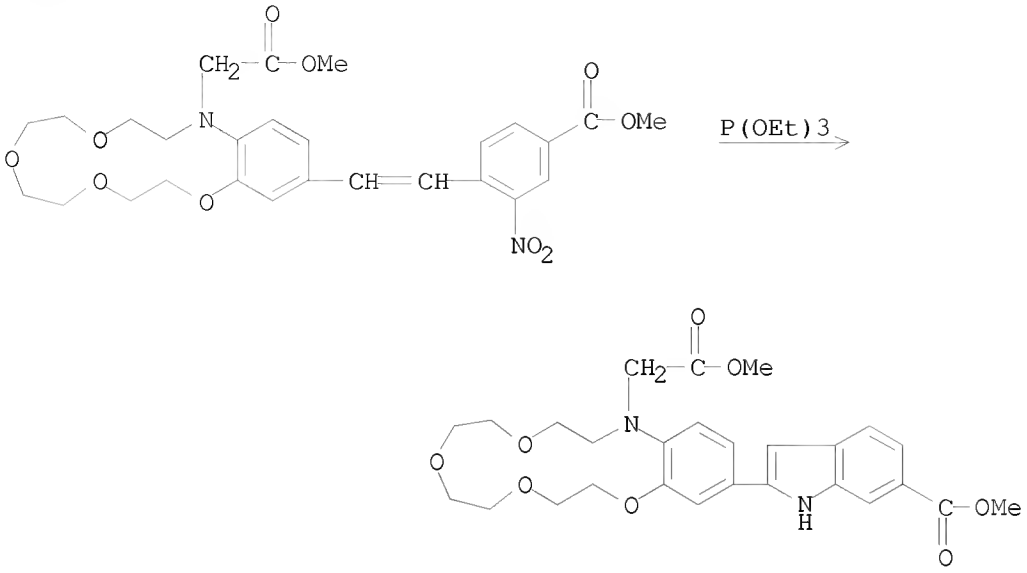
RX(54) OF 555



16%

REF: PCT Int. Appl., 136 pp.; 2005
CON: 16 hours, 120 deg C

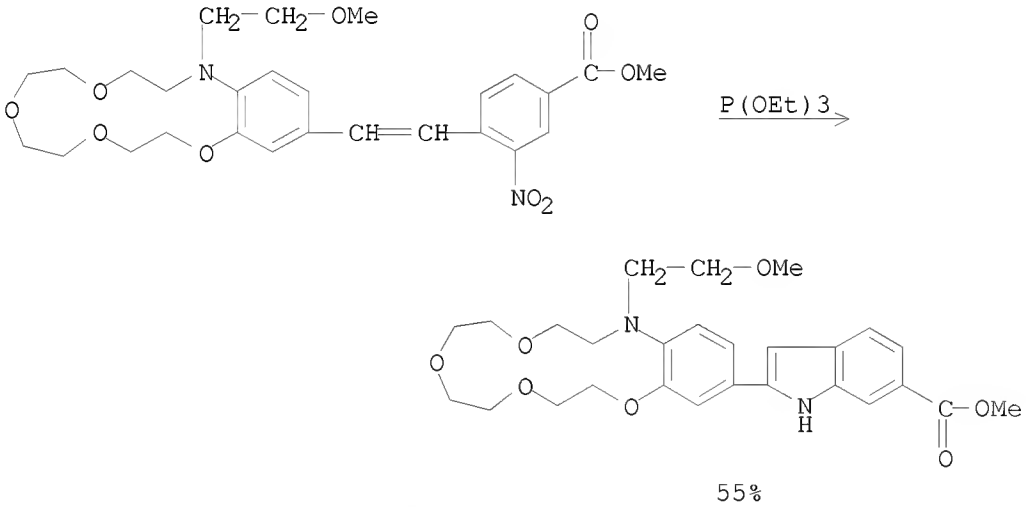
RX(67) OF 555



34%

REF: PCT Int. Appl., 136 pp.; 2005
CON: 4 hours, 125 deg C

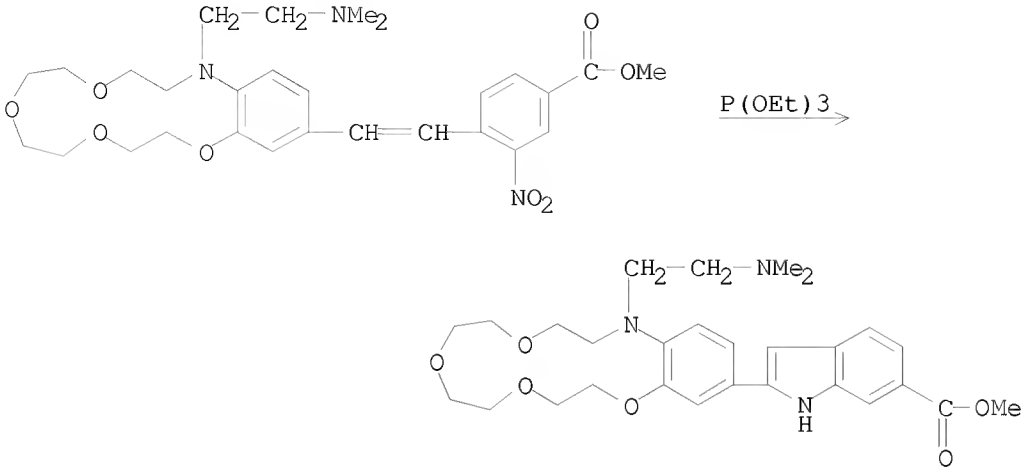
RX(91) OF 555



55%

REF: PCT Int. Appl., 136 pp.; 2005
CON: 4 hours, 125 deg C

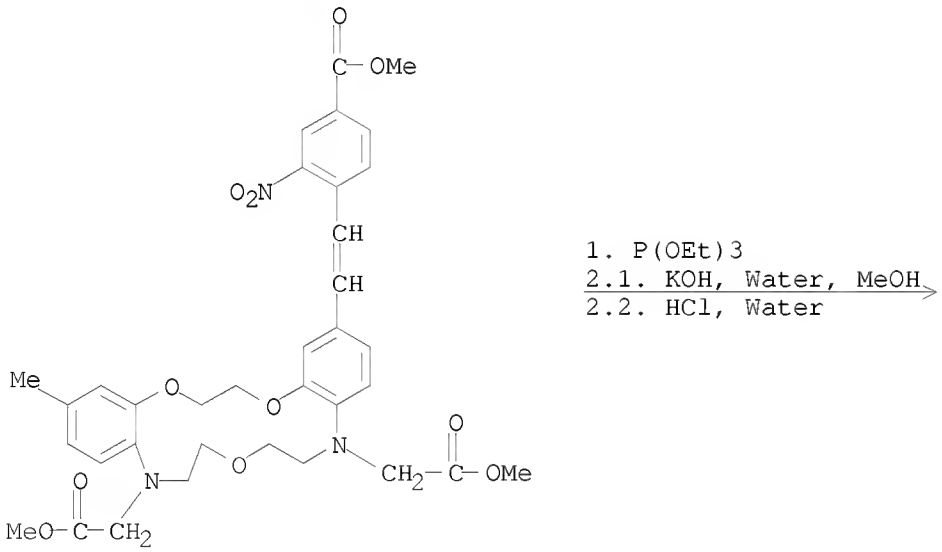
RX(97) OF 555



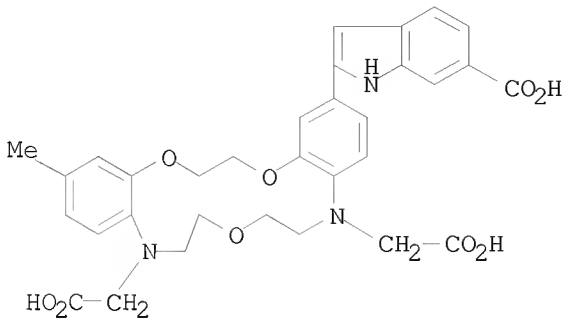
57%

REF: PCT Int. Appl., 136 pp.; 2005
CON: 14 hours, 125 deg C

RX(132) OF 555 - 2 STEPS



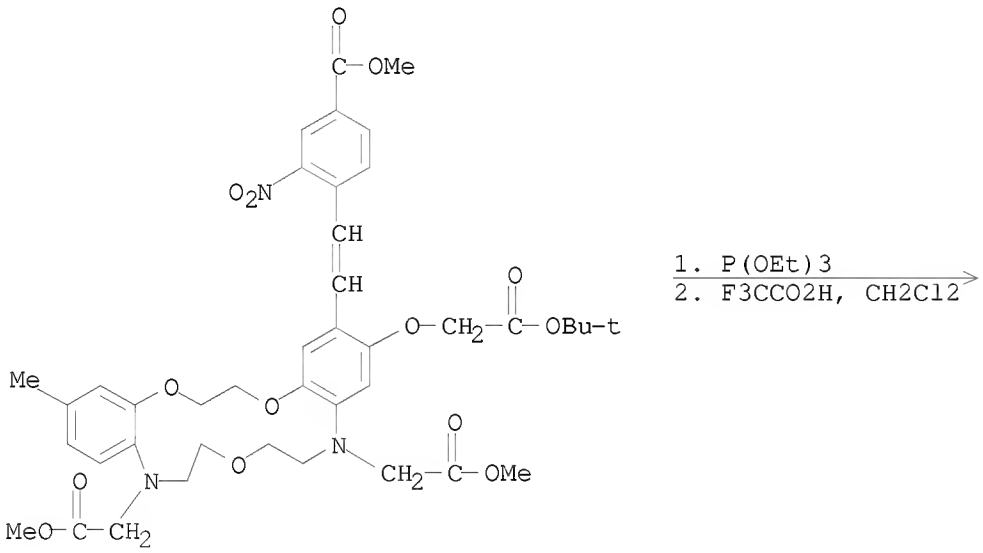
RX(132) OF 555 - 2 STEPS



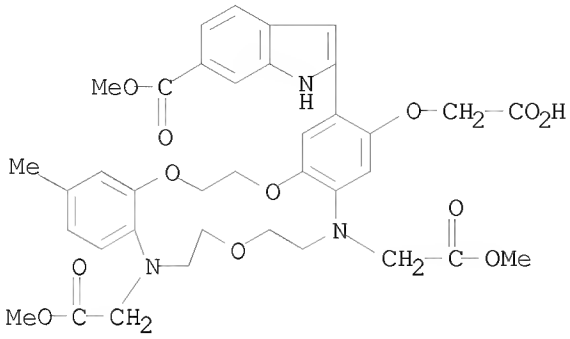
57%

REF: PCT Int. Appl., 136 pp.; 2005
NOTE: 2) incremental addition of reagent in stage 1
CON: STEP(1) 6 hours, 120 deg C
STEP(2.1) 22 hours, room temperature
STEP(2.2) room temperature, pH 3

RX(151) OF 555 - 2 STEPS



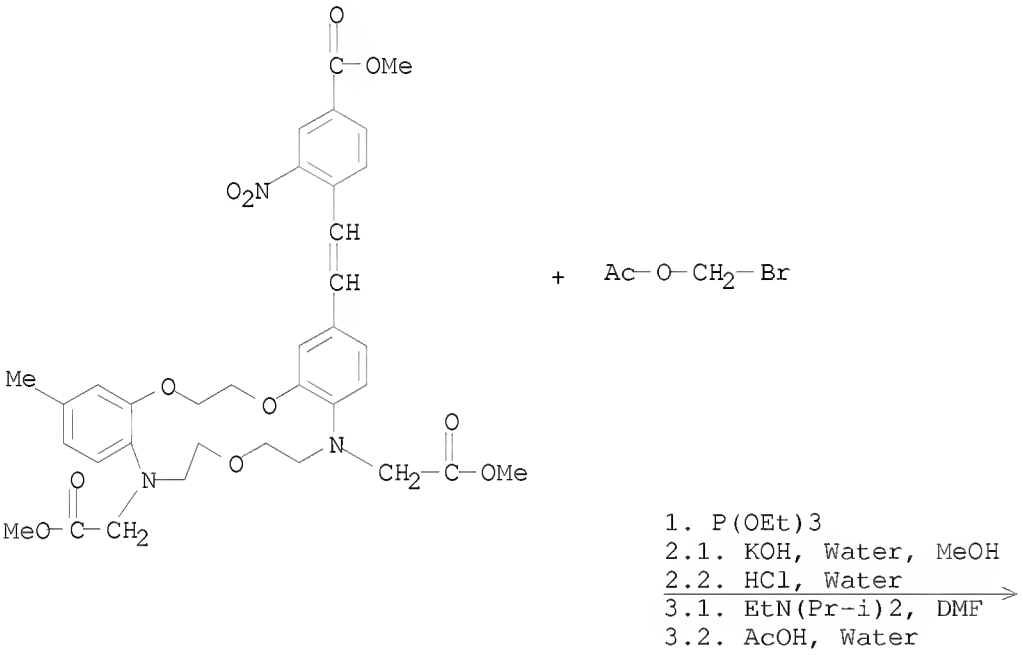
RX(151) OF 555 - 2 STEPS



57%

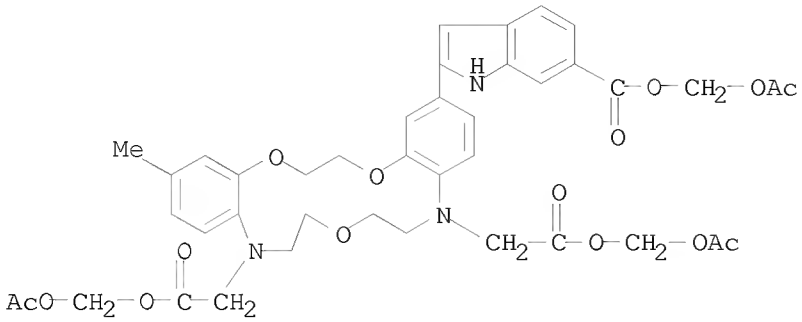
REF: PCT Int. Appl., 136 pp.; 2005
CON: STEP(1) 7 hours, 130 deg C
STEP(2) 3 hours, room temperature

RX(270) OF 555 - 3 STEPS



1. P(OEt)3
2.1. KOH, Water, MeOH
2.2. HCl, Water
3.1. EtN(Pr-i)2, DMF
3.2. AcOH, Water

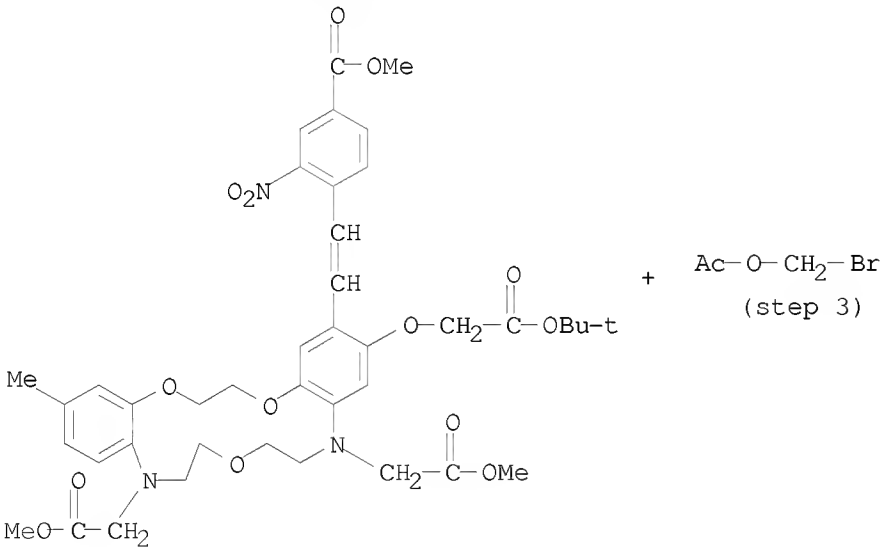
RX(270) OF 555 - 3 STEPS



3%

REF: PCT Int. Appl., 136 pp.; 2005
NOTE: 2) incremental addition of reagent in stage 1
CON: STEP(1) 6 hours, 120 deg C
STEP(2.1) 22 hours, room temperature
STEP(2.2) room temperature, pH 3
STEP(3.1) 16 hours, room temperature
STEP(3.2) room temperature

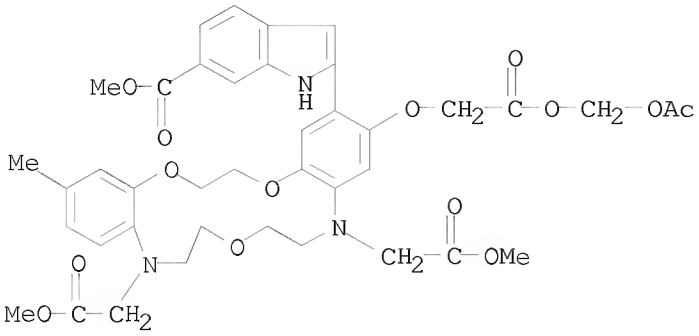
RX(300) OF 555 - 3 STEPS



(step 3)

1. P(OEt)3
2. F3CCO2H, CH2Cl2
3. EtN(Pr-i)2, DMF

RX(300) OF 555 - 3 STEPS

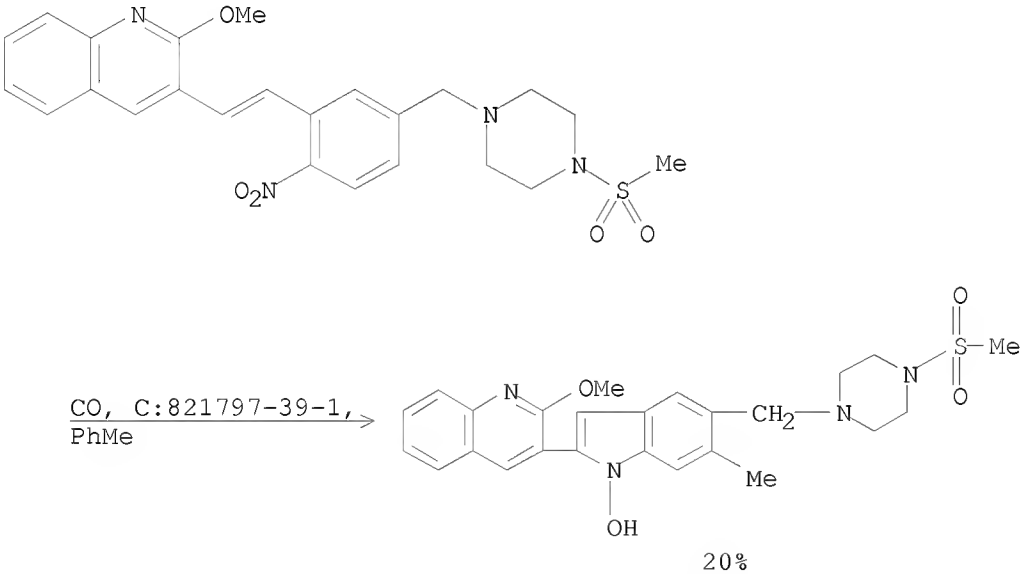


67%

REF: PCT Int. Appl., 136 pp.; 2005
CON: STEP(1) 7 hours, 130 deg C
STEP(2) 3 hours, room temperature
STEP(3) 16 hours, room temperature

L4 ANSWER 7 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

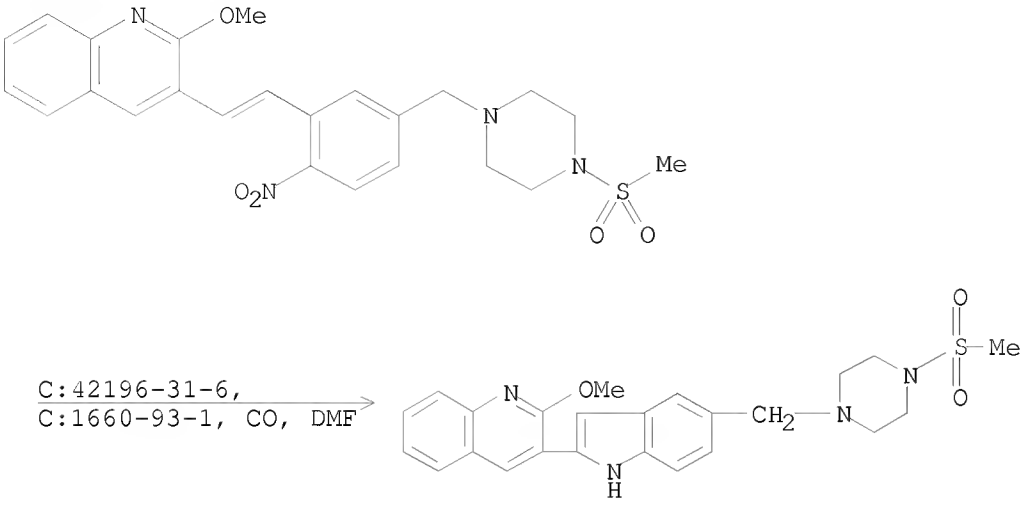
RX(5) OF 30



20%

REF: PCT Int. Appl., 2005000804, 06 Jan 2005
NOTE: Endeavor reactor was used
CON: STAGE(1) room temperature, 15 psi; 16 hours, 70 deg C

RX(6) OF 30

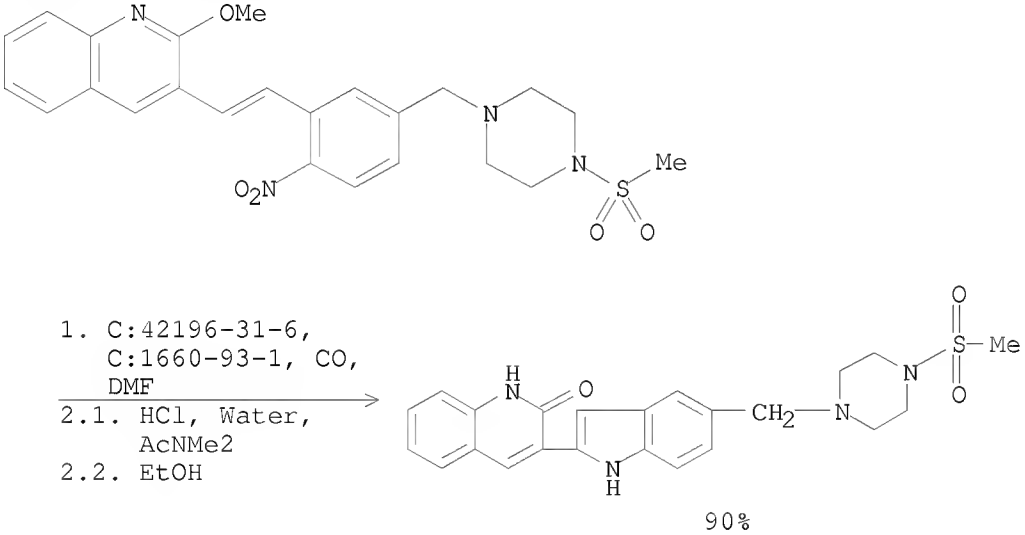


C:42196-31-6,
C:1660-93-1, CO, DMF

83%

REF: PCT Int. Appl., 31 pp.; 2005
CON: STAGE(1) room temperature, 15 psi; 14 hours, 70 deg C

RX(13) OF 30 - 2 STEPS



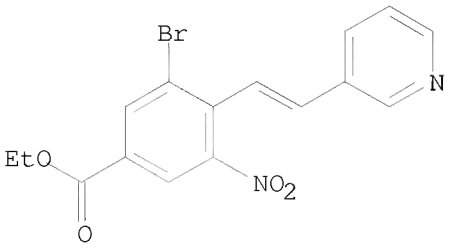
1. C:42196-31-6,
C:1660-93-1, CO,
DMF
2.1. HCl, Water,
AcNMe2
2.2. EtOH

90%

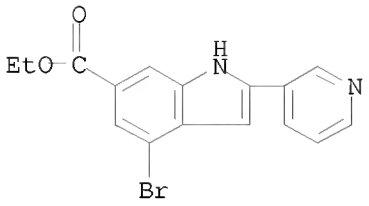
REF: PCT Int. Appl., 31 pp.; 2005
CON: STEP(1.1) room temperature, 15 psi; 14 hours, 70 deg C
STEP(2.1) 2 hours; 60 deg C

L4 ANSWER 8 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(37) OF 85



(step 1)

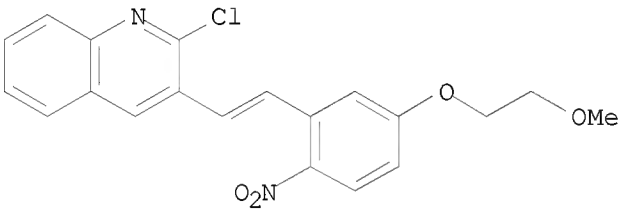


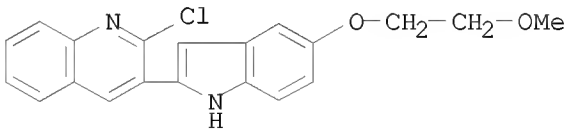
70%

REF: Chemistry--A European Journal, 9(21), 5323-5331; 2003
CON: 30 minutes, -40 deg C

L4 ANSWER 9 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 63

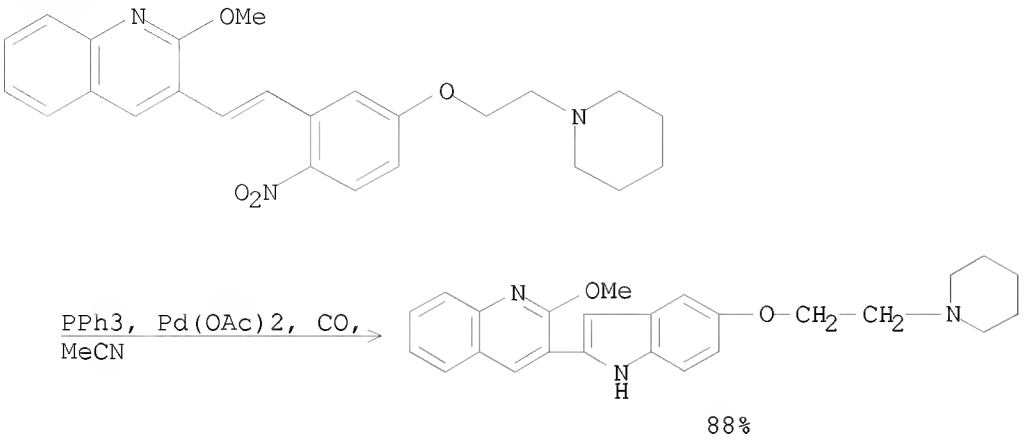




94%

REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

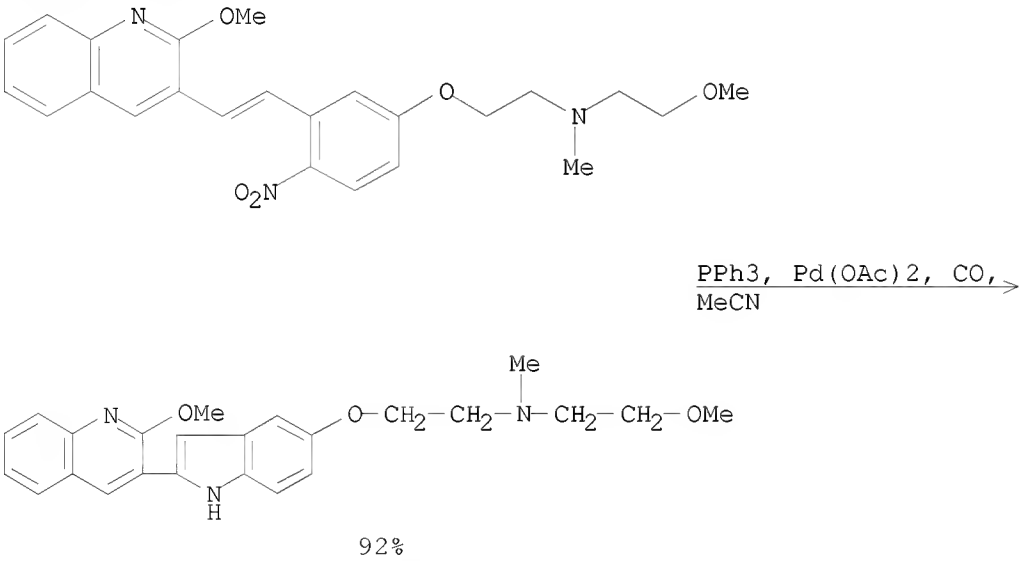
RX(10) OF 63



88%

REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

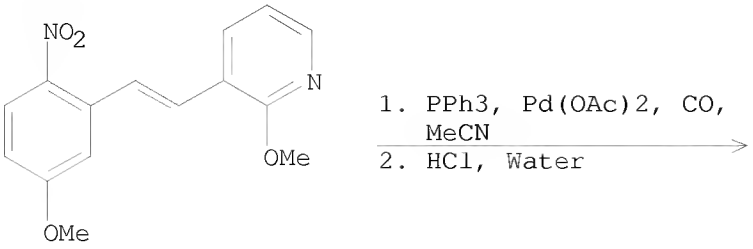
RX(15) OF 63



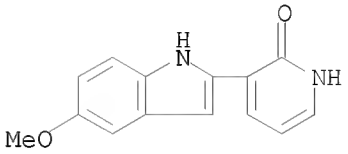
92%

REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: alternative prepn. shown
CON: 12 hours, 70 deg C, 6 atm

RX(17) OF 63



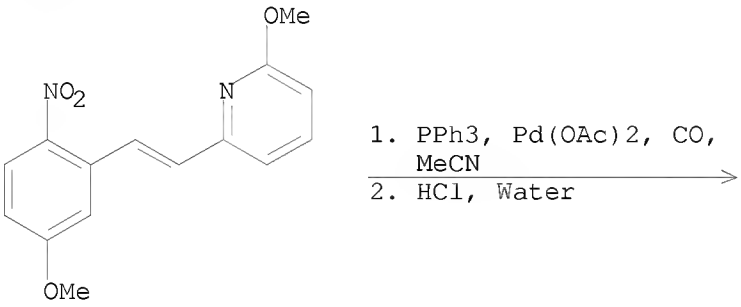
(step 1)



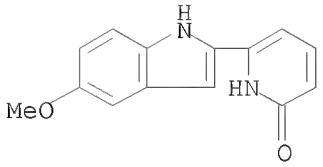
83%

REF: Organic Letters, 5(21), 3975-3978; 2003
CON: STAGE(1) 12 hours, 70 deg C, 6 atm
STAGE(2) 12 hours, reflux

RX(18) OF 63



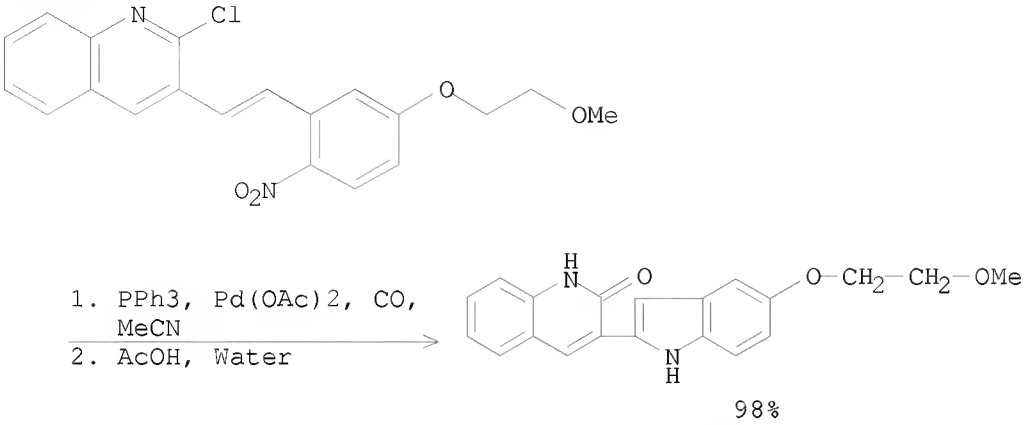
(step 1)



82%

REF: Organic Letters, 5(21), 3975-3978; 2003
CON: STAGE(1) 12 hours, 70 deg C, 6 atm
STAGE(2) 12 hours, reflux

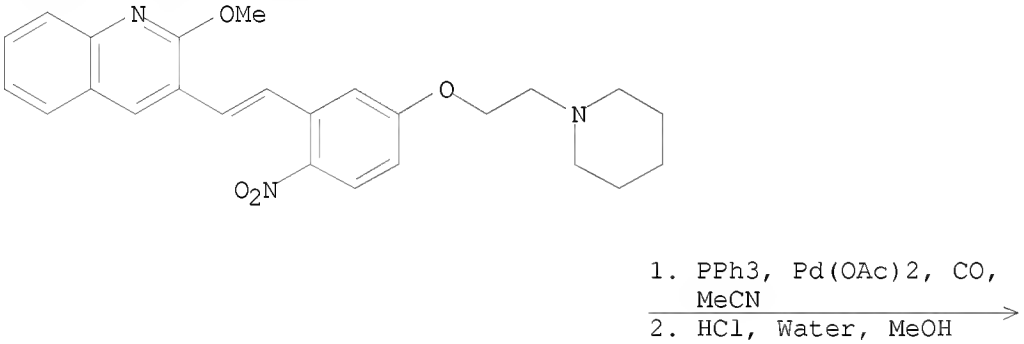
RX(25) OF 63 - 2 STEPS



98%

REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: 1) alternative prepn. shown, 2) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 3 hours, reflux

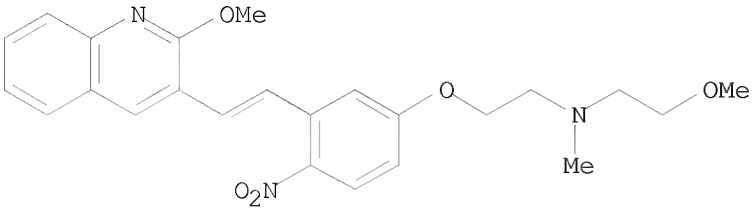
RX(29) OF 63 - 2 STEPS



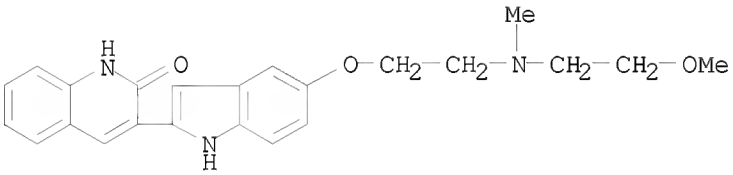
63%

REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: 1) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 4 hours, reflux

RX(33) OF 63 - 2 STEPS



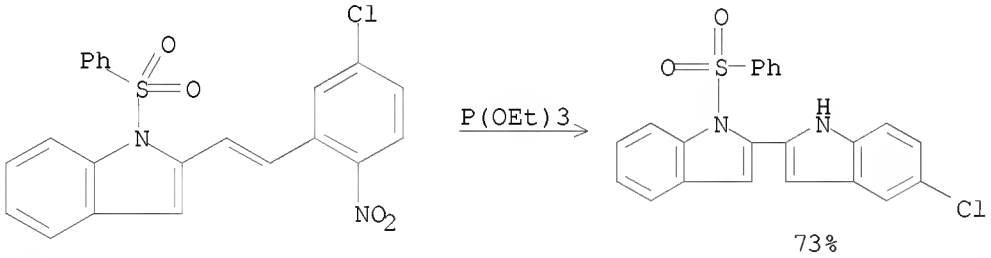
1. PPh3, Pd(OAc)2, CO, MeCN
2. HCl, Water, MeOH



REF: Organic Letters, 5(21), 3975-3978; 2003
NOTE: 1) alternative prepn. shown
CON: STEP(1) 12 hours, 70 deg C, 6 atm
STEP(2) 4 hours, reflux

L4 ANSWER 10 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 71

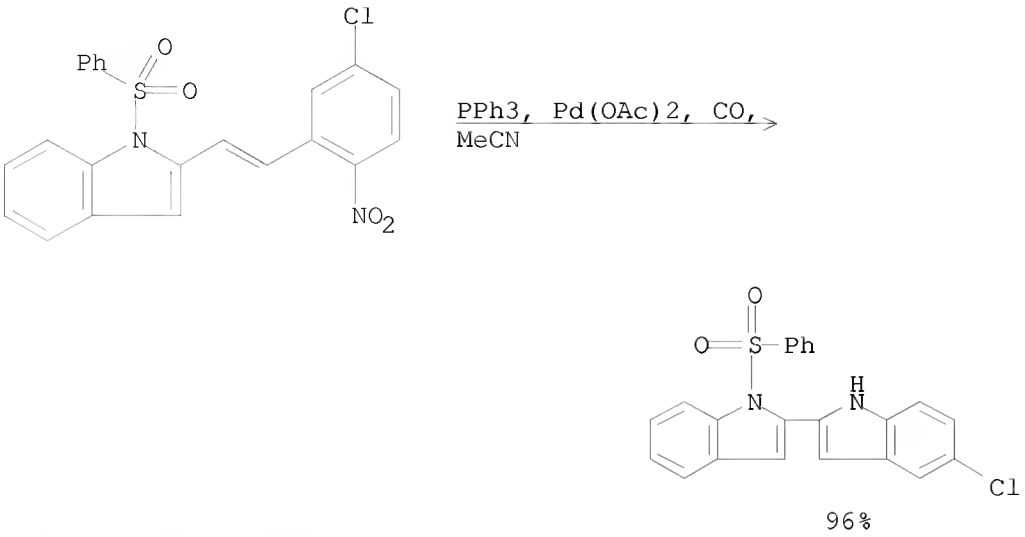


P(OEt)3

73%

REF: Organic Letters, 5(20), 3721-3723; 2003
CON: 2 hours, 155 deg C

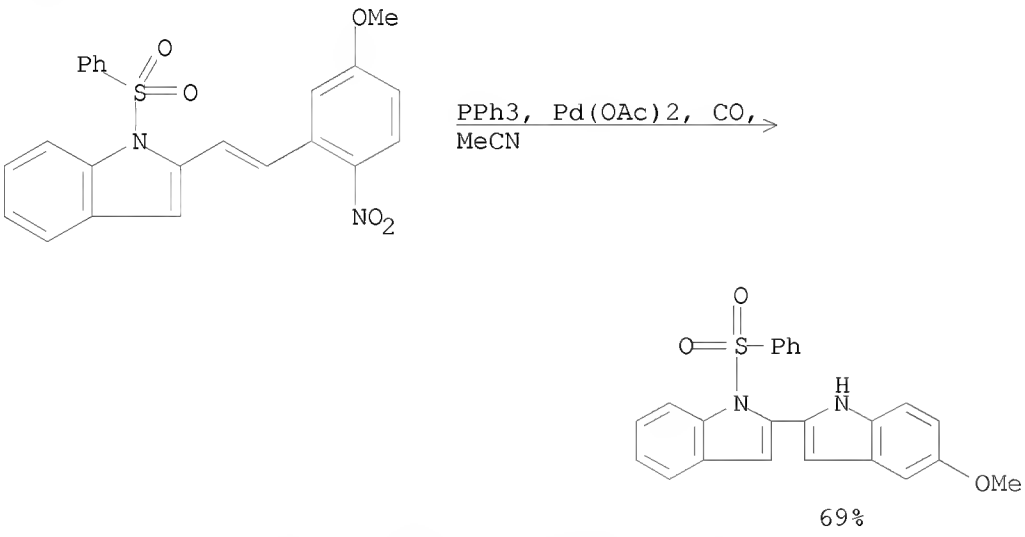
RX(4) OF 71



96%

REF: Organic Letters, 5(20), 3721-3723; 2003
CON: 12 hours, 70 deg C

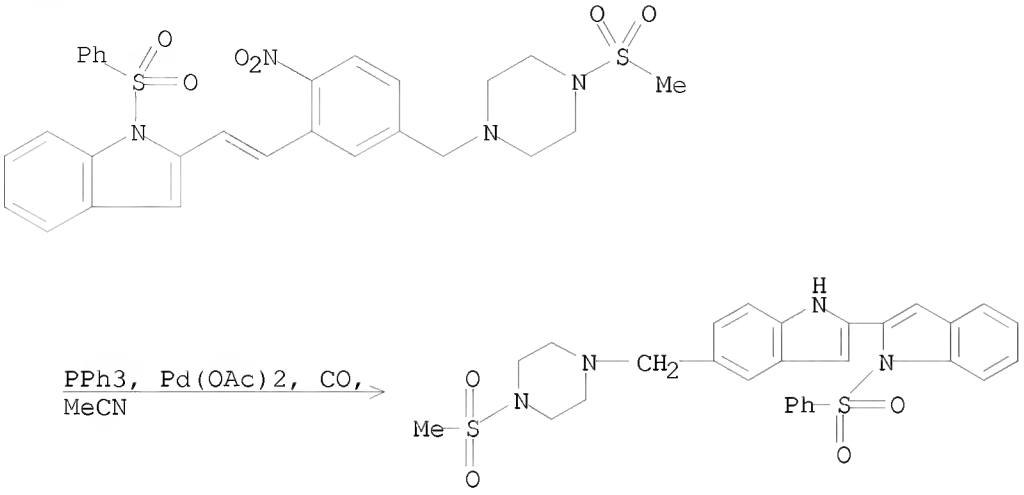
RX(6) OF 71



69%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

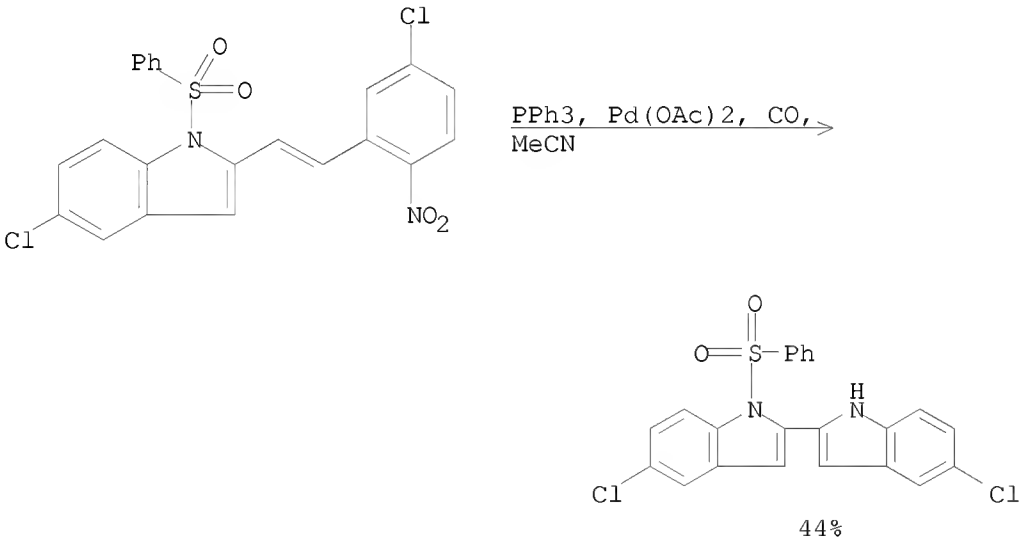
RX(7) OF 71



63%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

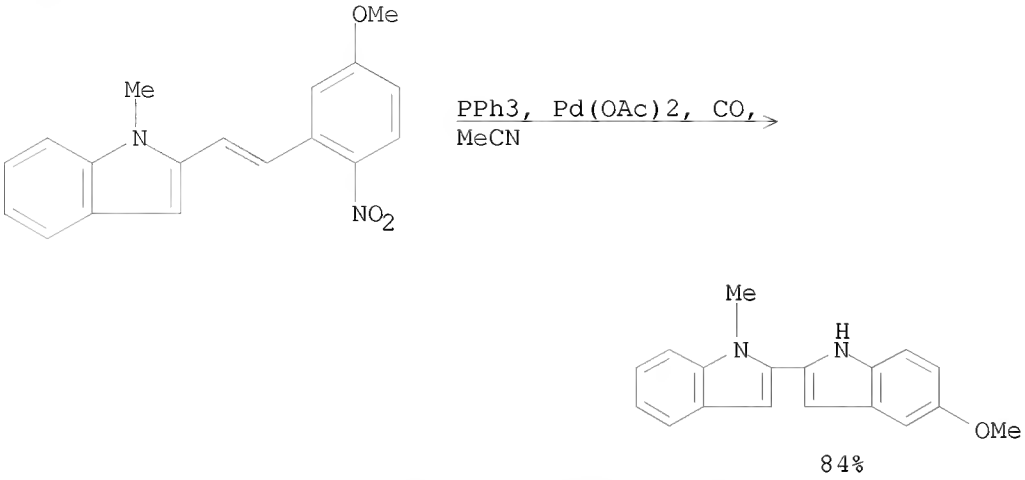
RX(9) OF 71



44%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

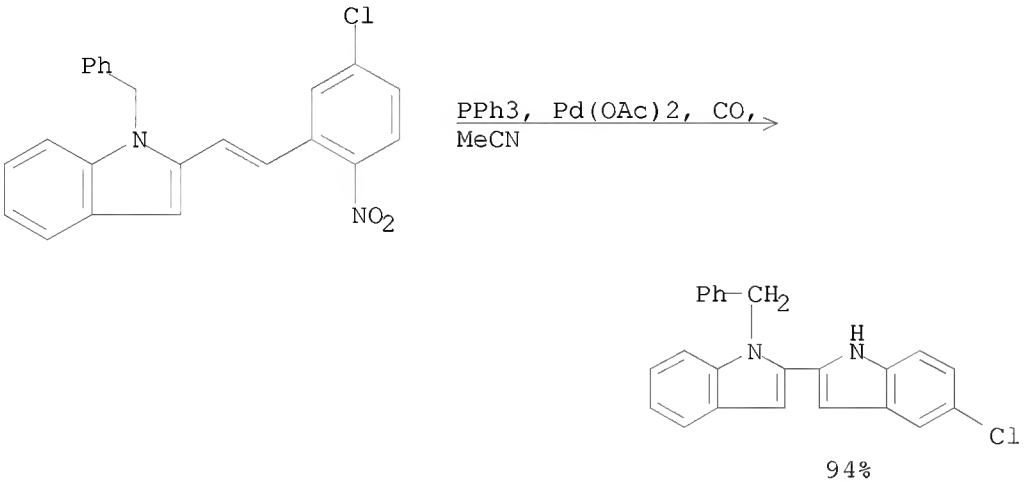
RX(11) OF 71



84%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

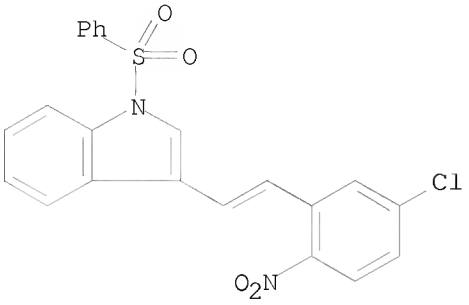
RX(14) OF 71



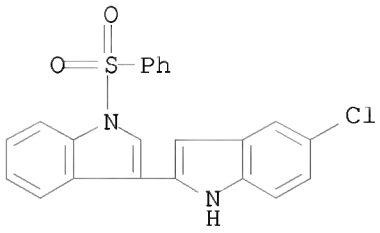
94%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

RX(16) OF 71



PPh3, Pd(OAc)2, CO,
MeCN

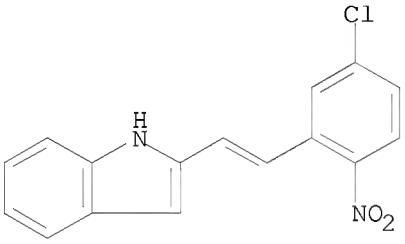


71%

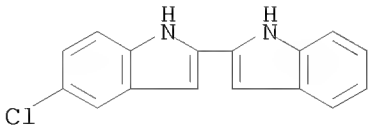
REF: Organic Letters, 5(20), 3721-3723; 2003

NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

RX(18) OF 71



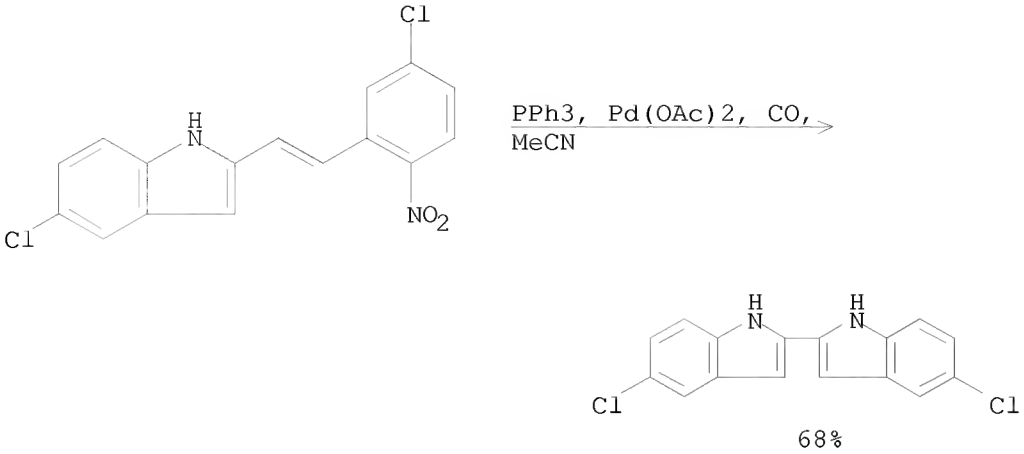
PPh3, Pd(OAc)2, CO,
MeCN



68%

REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

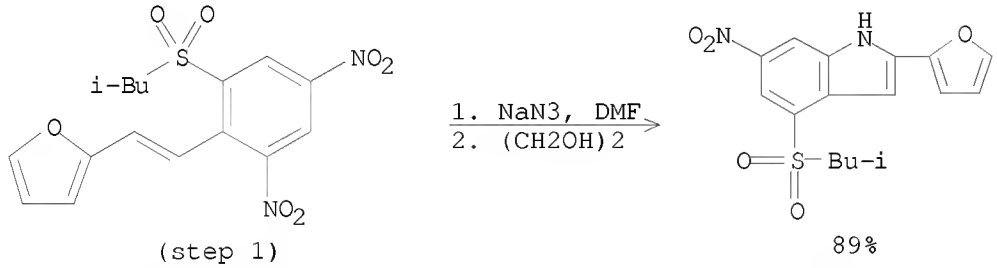
RX(21) OF 71



REF: Organic Letters, 5(20), 3721-3723; 2003
NOTE: using other method also got good yield
CON: 12 hours, 70 deg C

L4 ANSWER 11 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(11) OF 29

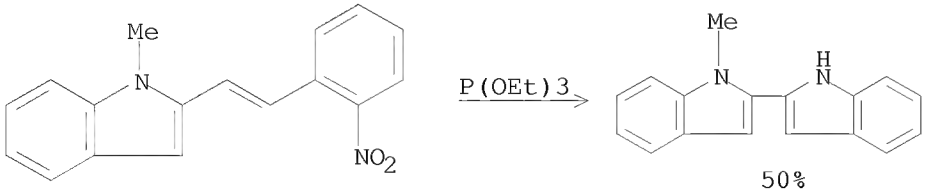


(step 1)

REF: Synthetic Communications, 32(9), 1465-1474; 2002
NOTE: regioselective, thermal, stereoselective

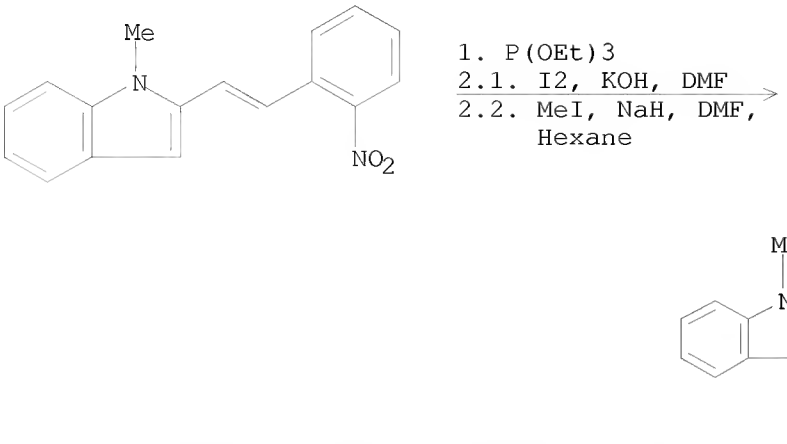
L4 ANSWER 12 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 177



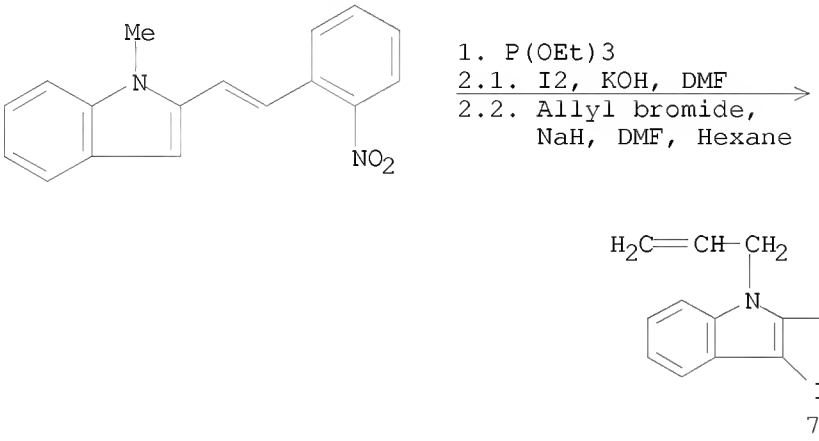
REF: Tetrahedron, 57(24), 5199-5212; 2001
NOTE: thermal, alternative prepns. gave similar yields

RX(43) OF 177 - 2 STEPS



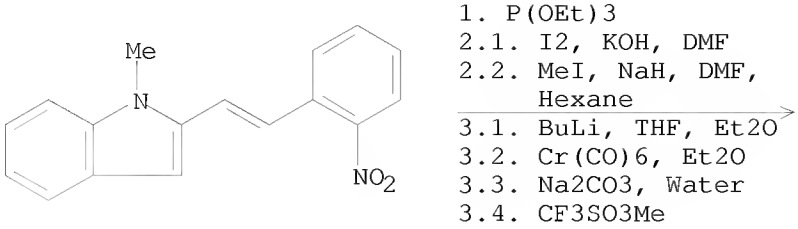
REF: Tetrahedron, 57(24), 5199-5212; 2001
NOTE: 1) thermal, alternative prepns. gave similar yields

RX(44) OF 177 - 2 STEPS

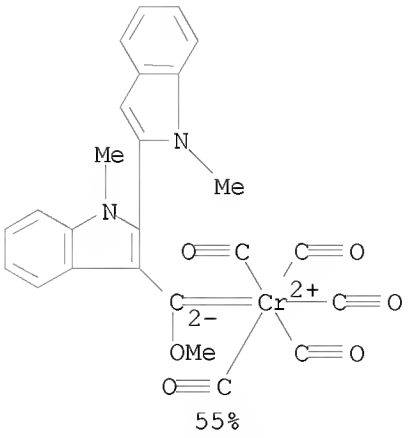


REF: Tetrahedron, 57(24), 5199-5212; 2001
NOTE: 1) thermal, alternative prepns. gave similar yields, 2) reactant assumed

RX(79) OF 177 - 3 STEPS

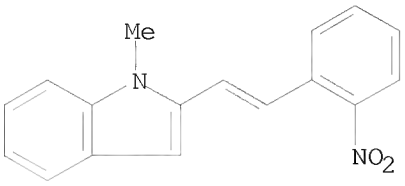


RX(79) OF 177 - 3 STEPS

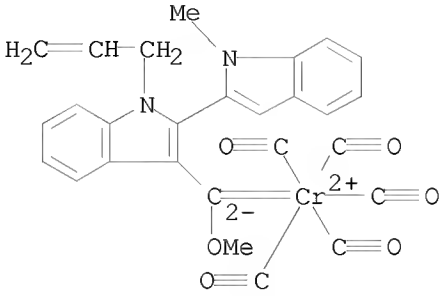


REF: Tetrahedron, 57(24), 5199-5212; 2001
NOTE: 1) thermal, alternative prepns. gave similar yields

RX(80) OF 177 - 3 STEPS



1. P(OEt)3
2.1. I2, KOH, DMF
2.2. Allyl bromide, NaH, DMF, Hexane
3.1. BuLi, THF, Et2O
3.2. Cr(CO)6, Et2O
3.3. Na2CO3, Water
3.4. CF3SO3Me

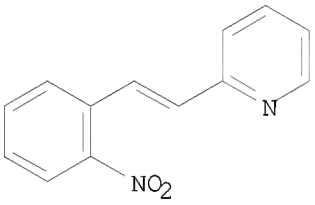


33%

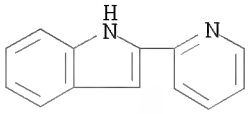
REF: Tetrahedron, 57(24), 5199-5212; 2001
NOTE: 1) thermal, alternative prepns. gave similar yields, 2) reactant assumed

L4 ANSWER 13 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

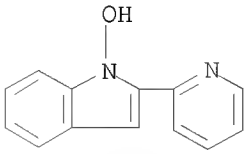
RX(4) OF 5



C:117686-64-3, CO, THF



29%

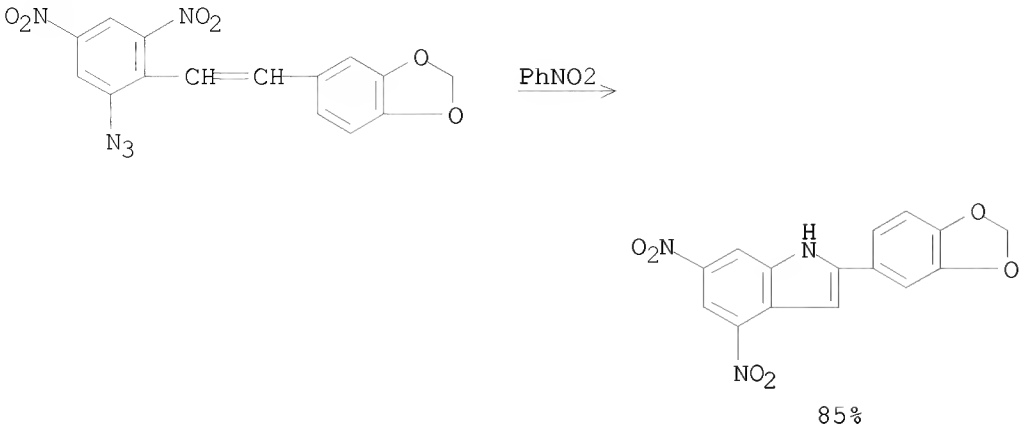


38%

REF: Journal of Molecular Catalysis A: Chemical, 152(1-2), 47-54; 2000

L4 ANSWER 14 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(22) OF 57



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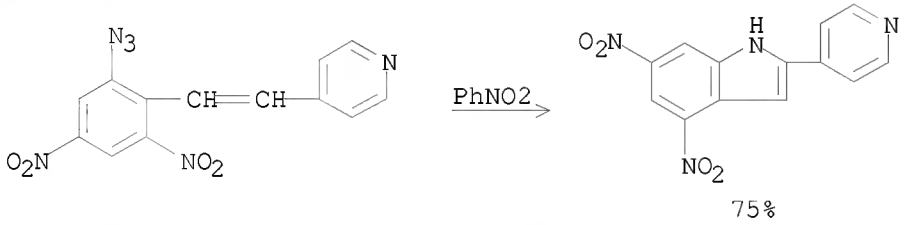
REF: Synthesis, (12), 2065-2070; 1999

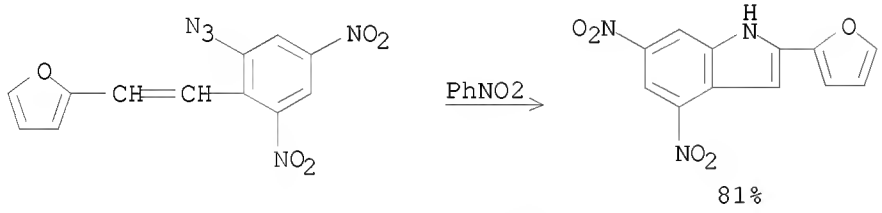
RX(24) OF 57



75%

REF: Synthesis, (12), 2065-2070; 1999

RX(25) OF 57



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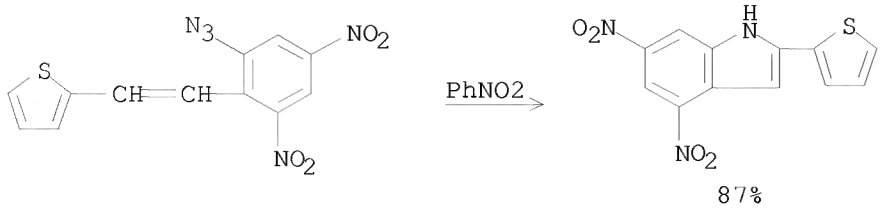
REF: Synthesis, (12), 2065-2070; 1999

RX(26) OF 57



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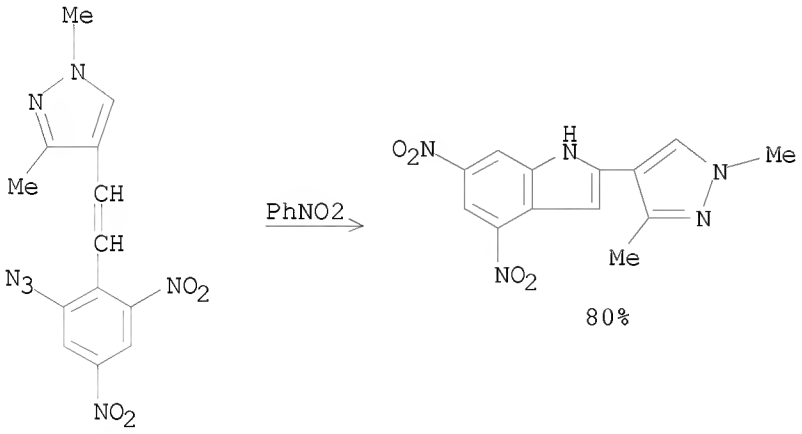
REF: Synthesis, (12), 2065-2070; 1999

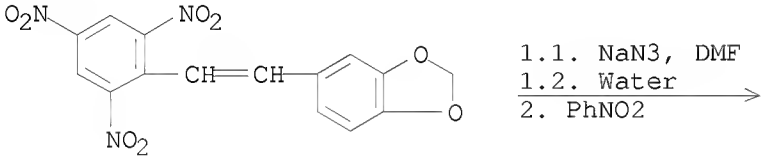
RX(28) OF 57

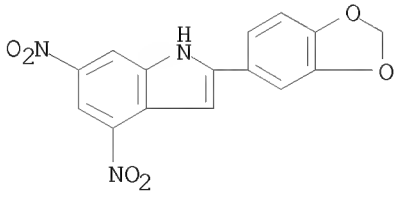


80%

REF: Synthesis, (12), 2065-2070; 1999

RX(41) OF 57 - 2 STEPS





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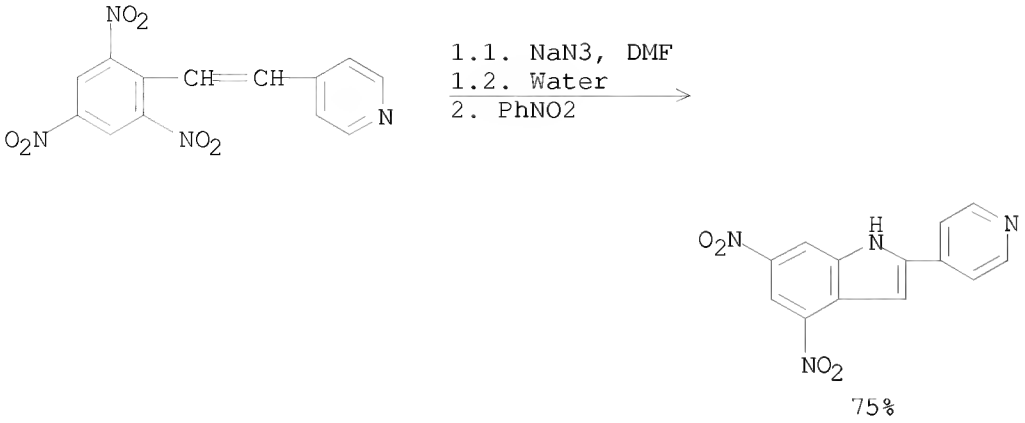
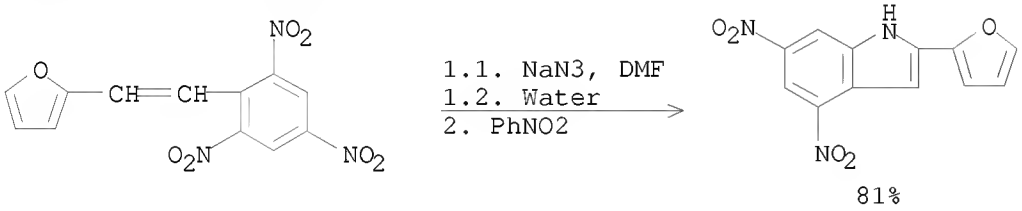
REF: Synthesis, (12), 2065-2070; 1999

RX(43) OF 57 - 2 STEPS



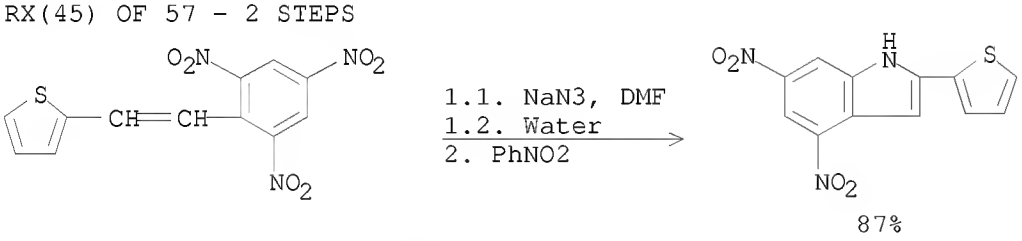
REF: Synthesis, (12), 2065-2070; 1999

RX(44) OF 57 - 2 STEPS



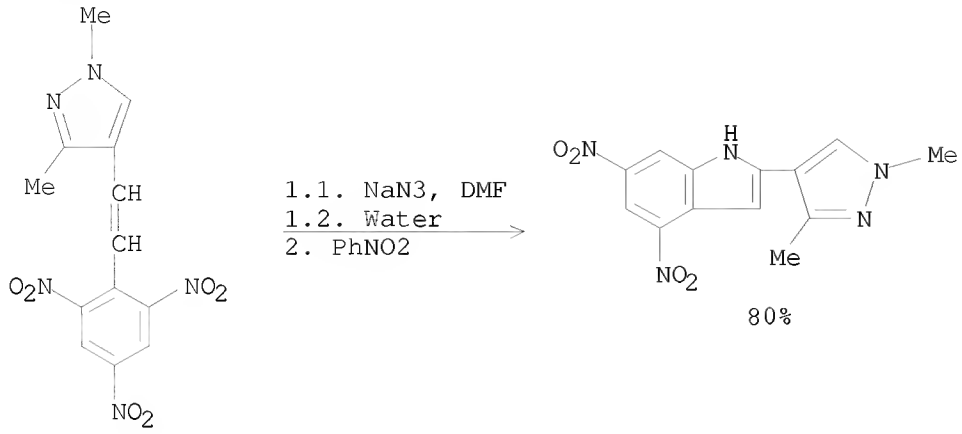
REF: Synthesis, (12), 2065-2070; 1999

RX(45) OF 57 - 2 STEPS



REF: Synthesis, (12), 2065-2070; 1999

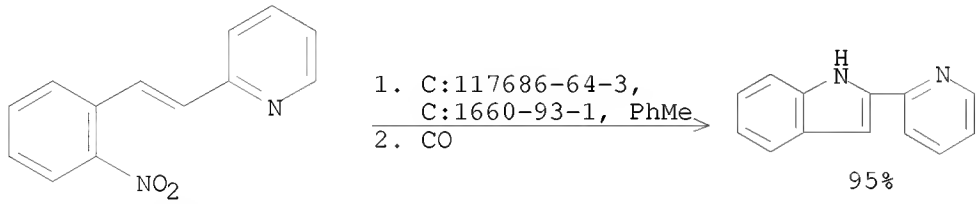
RX(47) OF 57 - 2 STEPS



REF: Synthesis, (12), 2065-2070; 1999

L4 ANSWER 15 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

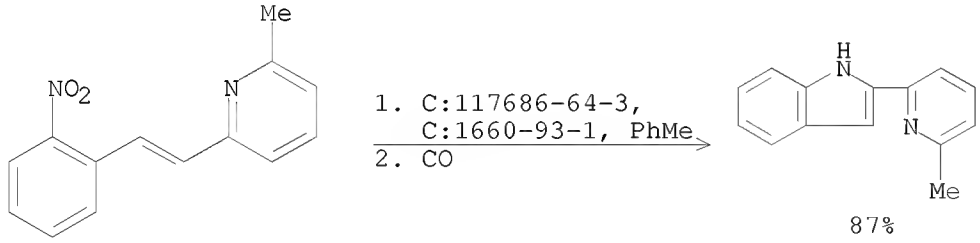
RX(1) OF 9



(step 1)

REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

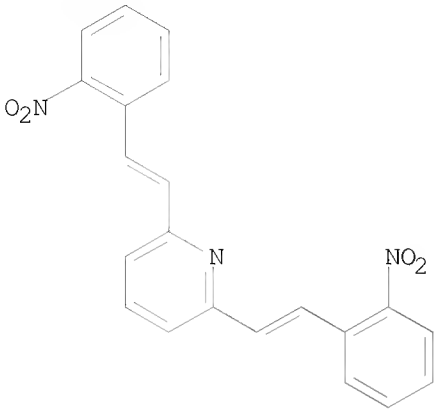
RX(2) OF 9



(step 1)

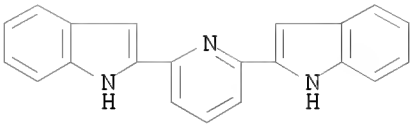
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(3) OF 9



1. C:117686-64-3,
   C:1660-93-1, PhMe
2. CO

(step 1)



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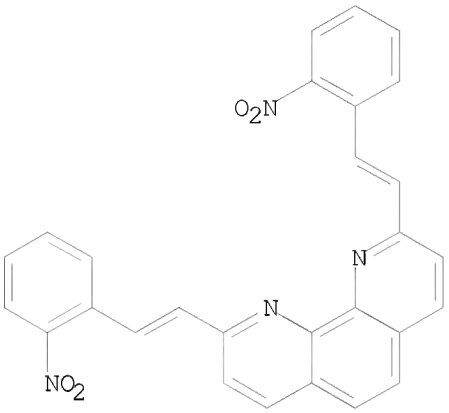
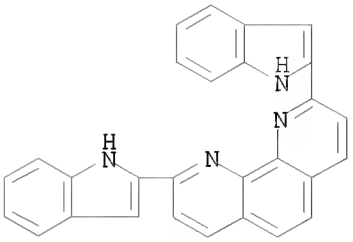
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(4) OF 9



(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



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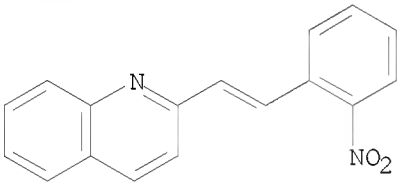
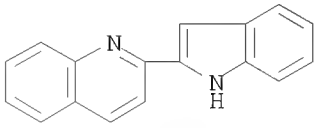
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(5) OF 9



(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



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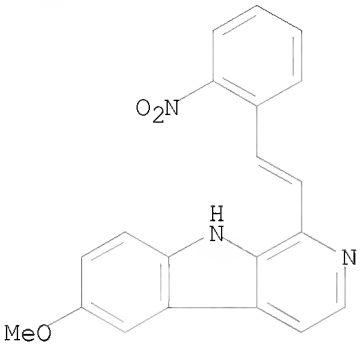
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(6) OF 9



(step 1)

1. C:117686-64-3,
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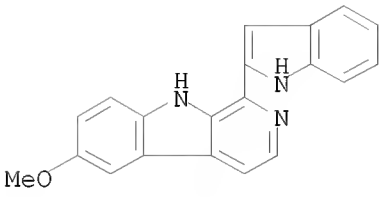
2. CO



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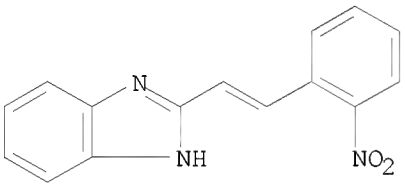
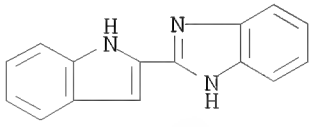
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(7) OF 9



(step 1)

1. C:117686-64-3,
   C:1660-93-1, PhMe
2. CO



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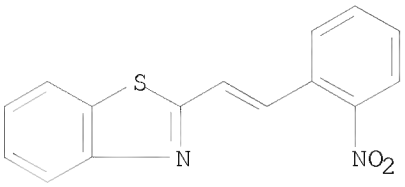
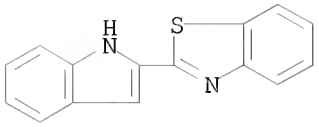
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(8) OF 9



(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



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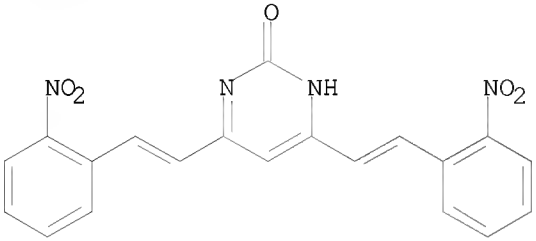
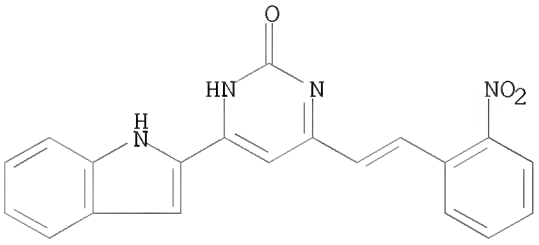
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

RX(9) OF 9



(step 1)

1. C:117686-64-3, C:1660-93-1, PhMe
2. CO



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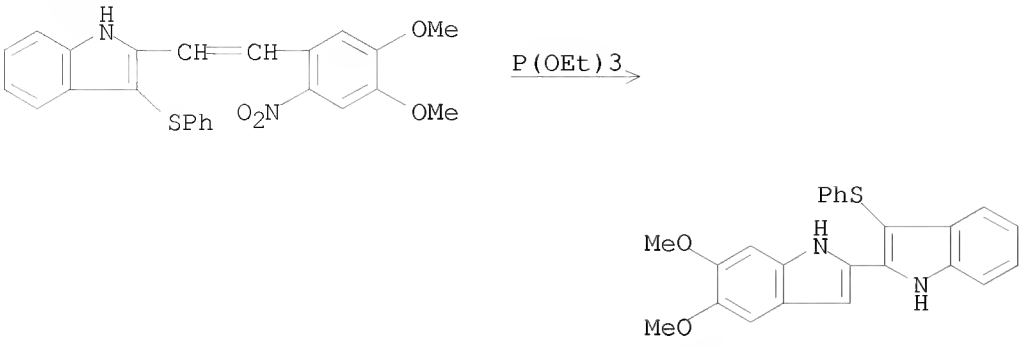
REF: Journal of Molecular Catalysis A: Chemical, 135(3), 241-248; 1998

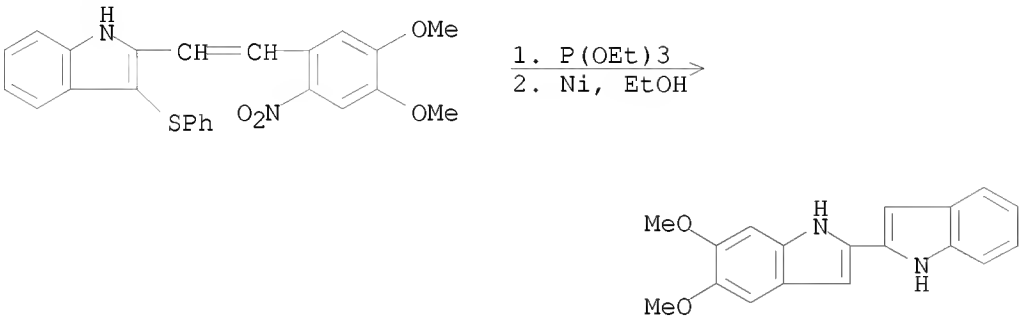
L4 ANSWER 16 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 6



REF: Synthetic Communications, 24(12), 1701-8; 1994

RX(5) OF 6 - 2 STEPS



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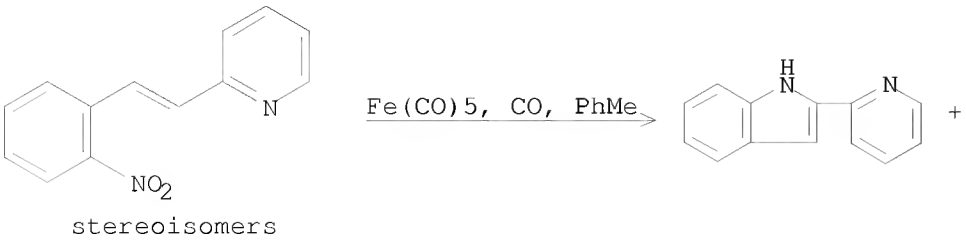
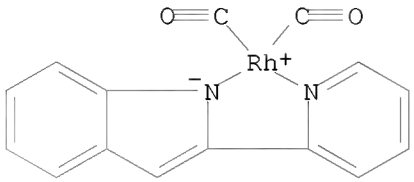
L4 ANSWER 17 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(8) OF 12



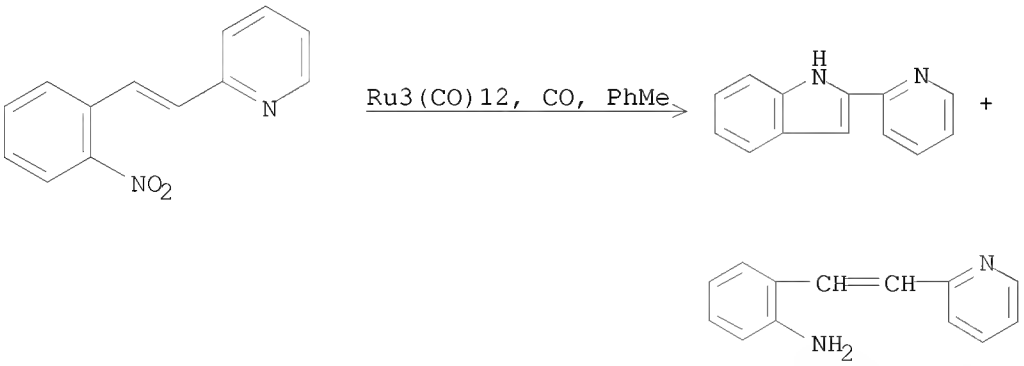
stereoisomers

RX(8) OF 12



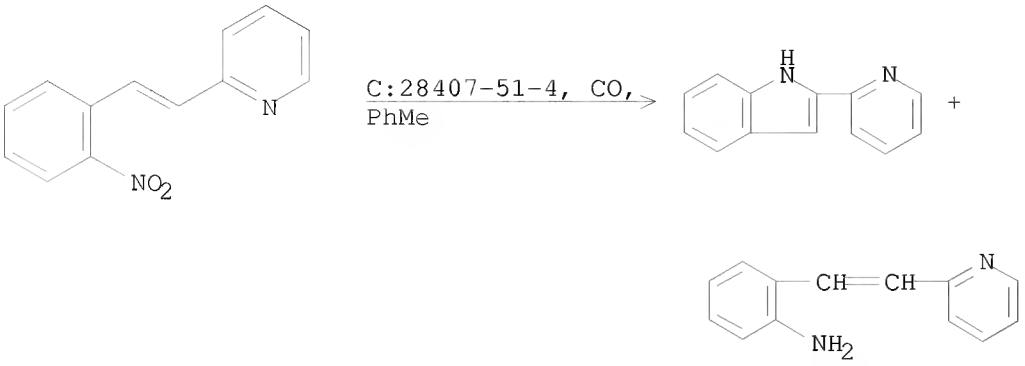
REF: Journal of the Chemical Society, Chemical Communications, (10), 784-6; 1986

RX(9) OF 12



REF: Journal of the Chemical Society, Chemical Communications, (10), 784-6; 1986

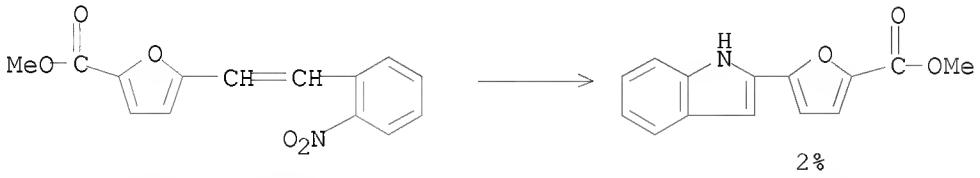
RX(10) OF 12



REF: Journal of the Chemical Society, Chemical Communications, (10), 784-6; 1986

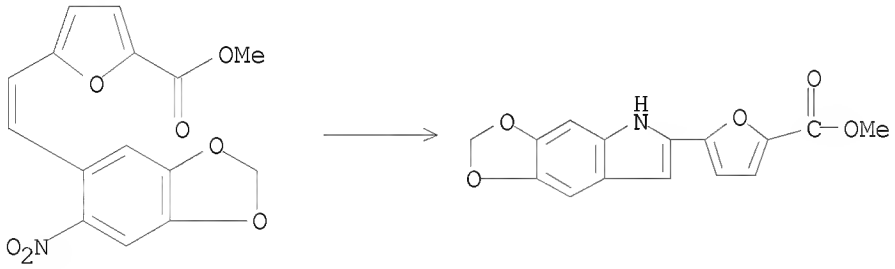
L4 ANSWER 18 OF 18 CASREACT COPYRIGHT 2008 ACS on STN

RX(69) OF 98 - 3 STEPS



REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

RX(72) OF 98 - 3 STEPS



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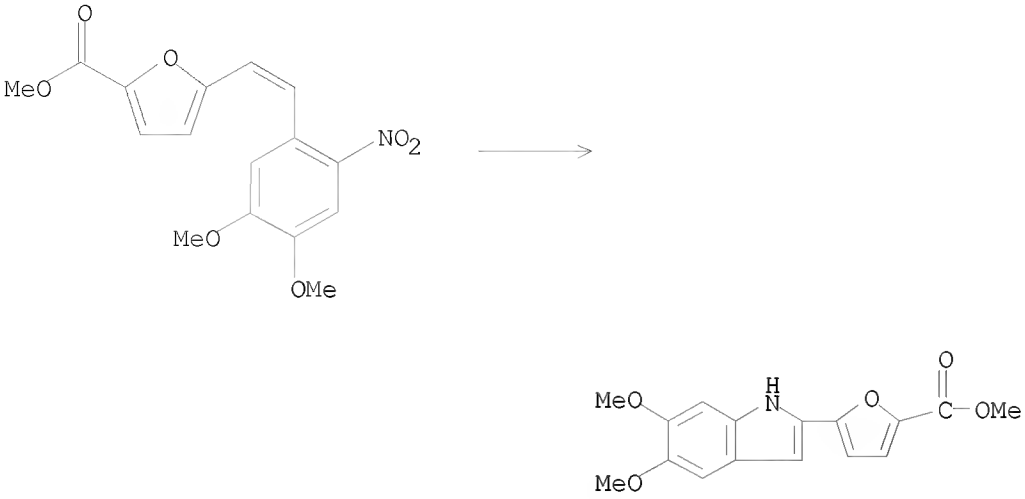
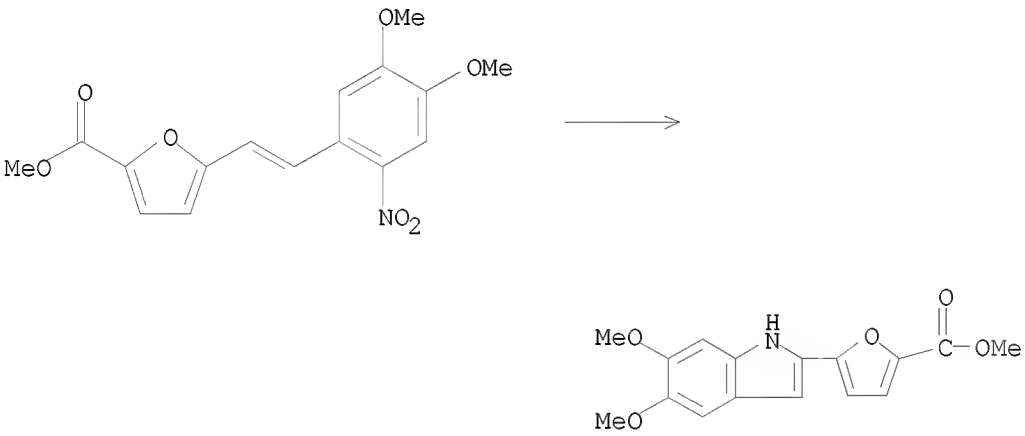


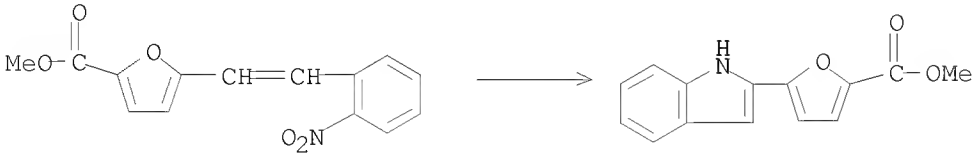
REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

RX(76) OF 98 - 3 STEPS



REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

RX(80) OF 98 - 4 STEPS



REF: Chemical & Pharmaceutical Bulletin, 30(1), 140-51; 1982

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